

Toluene-D8

Other names:	(2H8)toluene Benzene-D5-, methyl-D3- C6D5CD3 Perdeuterotoluene
Inchi:	InChI=1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3/i1D3,2D,3D,4D,5D,6D
InchiKey:	YXFVVABEGXRONW-JGUCLWPXSA-N
Formula:	C7D8
SMILES:	Cc1cccc1
Mol. weight [g/mol]:	100.19
CAS:	2037-26-5

Physical Properties

Property code	Value	Unit	Source
gf	120.47	kJ/mol	Joback Method
hf	48.72	kJ/mol	Joback Method
hfus	7.93	kJ/mol	Joback Method
hvap	33.45	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.995		Crippen Method
mcvol	85.730	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
rinpol	751.60		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	751.60		NIST Webbook
tb	386.24	K	Joback Method
tc	597.75	K	Joback Method
tf	195.07	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.38	J/mol×K	597.75	Joback Method
cpg	149.61	J/mol×K	421.49	Joback Method

cpg	160.38	J/mol×K	456.74	Joback Method
cpg	170.51	J/mol×K	492.00	Joback Method
cpg	180.04	J/mol×K	527.25	Joback Method
cpg	188.99	J/mol×K	562.50	Joback Method
cpg	138.18	J/mol×K	386.24	Joback Method
dvisc	0.0028683	Pa×s	195.07	Joback Method
dvisc	0.0013935	Pa×s	226.93	Joback Method
dvisc	0.0008087	Pa×s	258.79	Joback Method
dvisc	0.0005288	Pa×s	290.65	Joback Method
dvisc	0.0003760	Pa×s	322.52	Joback Method
dvisc	0.0002843	Pa×s	354.38	Joback Method
dvisc	0.0002251	Pa×s	386.24	Joback Method
hvapt	37.95	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
tcondl	0.12	W/m×K	326.70	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	326.47	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	316.24	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	316.08	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	315.84	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	297.28	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	297.13	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	296.90	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	279.73	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	279.57	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	279.35	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	260.06	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	259.91	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	259.69	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	326.87	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	https://www.doi.org/10.1021/je034162x
Enthalpies of Vaporization and Vapor Pressures of Aromatics and Deuterated Hydrocarbons	https://www.doi.org/10.1021/je800091s
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Isotope Effects:	https://link.springer.com/article/10.1007/BF02311772
McGowan Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2037265&Units=SI
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2037265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume

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