Toluene-D3

Other names:	Benzene, trideuteromethyl-
	C6H5CD3
Inchi:	InChI=1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3/i1D3
InchiKey:	YXFVVABEGXRONW-FIBGUPNXSA-N
Formula:	C7H5D3
SMILES:	Cc1ccccc1
Mol. weight [g/mol]:	95.16
CAS:	1124-18-1

Physical Properties

Property code	Value	Unit	Source
affp	789.70	kJ/mol	NIST Webbook
basg	762.00	kJ/mol	NIST Webbook
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
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	138.18	J/mol×K	386.24	Joback Method
cpg	188.99	J/mol×K	562.50	Joback Method
cpg	180.04	J/mol×K	527.25	Joback Method
cpg	170.51	J/mol×K	492.00	Joback Method
cpg	160.38	J/mol×K	456.74	Joback Method

cpg	149.61	J/mol×K	421.49	Joback Method
cpg	197.38	J/mol×K	597.75	Joback Method
dvisc	0.0002251	Pa×s	386.24	Joback Method
dvisc	0.0002843	Pa×s	354.38	Joback Method
dvisc	0.0003760	Pa×s	322.52	Joback Method
dvisc	0.0005288	Pa×s	290.65	Joback Method
dvisc	0.0008087	Pa×s	258.79	Joback Method
dvisc	0.0013935	Pa×s	226.93	Joback Method
dvisc	0.0028683	Pa×s	195.07	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124181&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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