

1,2-Di(methyl-d3)benzene-d4

Other names:	(2H10)-o-xylene O-xylene-d10
Inchi:	InChI=1S/C8H10/c1-7-5-3-4-6-8(7)2/h3-6H,1-2H3/i1D3,2D3,3D,4D,5D,6D
InchiKey:	CTQNGGLPUBDAKN-ZGYYUIRESA-N
Formula:	C8D10
SMILES:	Cc1ccccc1C
Mol. weight [g/mol]:	116.23
CAS:	56004-61-6

Physical Properties

Property code	Value	Unit	Source
gf	119.26	kJ/mol	Joback Method
hf	16.61	kJ/mol	Joback Method
hfus	10.13	kJ/mol	Joback Method
hvap	43.00	kJ/mol	NIST Webbook
log10ws	-2.42		Crippen Method
logp	2.303		Crippen Method
mcvol	99.820	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
tb	414.10	K	Joback Method
tc	625.12	K	Joback Method
tf	218.86	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.89	J/mol×K	625.12	Joback Method
cpg	231.65	J/mol×K	589.95	Joback Method
cpg	221.85	J/mol×K	554.78	Joback Method
cpg	211.46	J/mol×K	519.61	Joback Method
cpg	200.48	J/mol×K	484.44	Joback Method
cpg	188.87	J/mol×K	449.27	Joback Method
cpg	176.61	J/mol×K	414.10	Joback Method

dvisc	0.0020700	Pa×s	218.86	Joback Method
dvisc	0.0002175	Pa×s	414.10	Joback Method
dvisc	0.0002698	Pa×s	381.56	Joback Method
dvisc	0.0003483	Pa×s	349.02	Joback Method
dvisc	0.0004740	Pa×s	316.48	Joback Method
dvisc	0.0006923	Pa×s	283.94	Joback Method
dvisc	0.0011152	Pa×s	251.40	Joback Method
hvapt	43.00	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56004616&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects:	https://www.doi.org/10.1021/je800091s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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