Hexamethylbenzene, deuterated

Other names: hexamethylbenzene-d18
Inchi: InChI=1S/C12H18/c1-7-8(2)10(4)12(6)11(5)9(7)3/h1-6H3/i1D3,2D3,3D3,4D3,5D3,6D3
InchiKey: YUWFEBAXEOLKSG-NBDUPMGQSA-N
Formula: C12D18
SMILES: Cc1c(C)c(C)c(C)c(C)c1C
Mol. weight [g/mol]: 180.38
CAS: 4342-40-9

Physical Properties

Property code	Value	Unit	Source
gf	114.42	kJ/mol	Joback Method
hf	-111.83	kJ/mol	Joback Method
hfus	18.93	kJ/mol	Joback Method
hvap	68.20	kJ/mol	NIST Webbook
log10ws	-4.33		Crippen Method
logp	3.537		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
ss	348.06	J/mol×K	NIST Webbook
tb	525.54	K	Joback Method
tc	730.53	K	Joback Method
tf	314.02	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.45	J/mol×K	696.36	Joback Method
cpg	347.90	J/mol×K	525.54	Joback Method
cpg	363.06	J/mol×K	559.70	Joback Method
cpg	377.58	J/mol×K	593.87	Joback Method
cpg	391.48	J/mol×K	628.03	Joback Method
cpg	404.77	J/mol×K	662.20	Joback Method
cpg	429.53	J/mol×K	730.53	Joback Method

cps	290.51	J/mol×K	300.00	NIST Webbook
dvisc	0.0001772	Pa×s	525.54	Joback Method
dvisc	0.0008438	Pa×s	314.02	Joback Method
dvisc	0.0005705	Pa×s	349.27	Joback Method
dvisc	0.0004145	Pa×s	384.53	Joback Method
dvisc	0.0003177	Pa×s	419.78	Joback Method
dvisc	0.0002538	Pa×s	455.03	Joback Method
dvisc	0.0002094	Pa×s	490.29	Joback Method
hvapt	68.23	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4342409&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

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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

ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume