Hexane-d14

Inchi: InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3/i1D3,2D3,3D2,4D2,5D2,6D2
InchiKey: VLKZOEOYAKHREP-ZLKPZJALSA-N
Formula: C6D14
SMILES: CCCCCC
Mol. weight [g/mol]: 100.26
CAS: 21666-38-6

Physical Properties

Property code	Value	Unit	Source
gf	-0.36	kJ/mol	Joback Method
hf	-167.17	kJ/mol	Joback Method
hfus	11.30	kJ/mol	Joback Method
hvap	28.95	kJ/mol	Joback Method
ie	10.18	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.587		Crippen Method
mcvol	95.400	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	589.00		NIST Webbook
tb	336.68	K	Joback Method
tc	499.98	K	Joback Method
tf	157.38	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.63	J/mol×K	336.68	Joback Method
cpg	169.08	J/mol×K	363.90	Joback Method
cpg	179.18	J/mol×K	391.11	Joback Method
cpg	188.94	J/mol×K	418.33	Joback Method
cpg	198.36	J/mol×K	445.54	Joback Method
cpg	207.45	J/mol×K	472.76	Joback Method
cpg	216.22	J/mol×K	499.98	Joback Method

dvisc	0.0044393	Pa×s	157.38	Joback Method
dvisc	0.0018274	Pa×s	187.26	Joback Method
dvisc	0.0009604	Pa×s	217.15	Joback Method
dvisc	0.0005897	Pa×s	247.03	Joback Method
dvisc	0.0004023	Pa×s	276.91	Joback Method
dvisc	0.0002957	Pa×s	306.80	Joback Method
dvisc	0.0002295	Pa×s	336.68	Joback Method
hvapt	31.59	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=C21666386&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
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume