heptane-d16

Other names: perdeuteroheptane
Inchi: InChI=1S/C7H16/c1-3-5-7-6-4-2/h3-7H2,1-2H3/i1D3,2D3,3D2,4D2,5D2,6D2,7D2
InchiKey: IMNFDUFMRHMDMM-NEBSKJCTSA-N
Formula: C7D16
SMILES: CCCCCCC
Mol. weight [g/mol]: 116.30
CAS: 33838-52-7

Physical Properties

Property code	Value	Unit	Source
af	0.3716		Cheméo Relay (1.0)
gf	8.06	kJ/mol	Joback Method
hf	-189.90	kJ/mol	Cheméo Relay (1.0)
hfus	13.89	kJ/mol	Joback Method
hvap	36.35	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
log10ws	-4.70		Cheméo Relay (1.0)
logp	2.977		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	379.34	K	Cheméo Relay (1.0)
tc	540.63	K	Cheméo Relay (1.0)
tf	192.72	K	Cheméo Relay (1.0)
vc	0.439	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.21	J/mol×K	359.56	Joback Method
cpg	259.03	J/mol×K	523.11	Joback Method
cpg	249.19	J/mol×K	495.85	Joback Method
cpg	238.97	J/mol×K	468.59	Joback Method
cpg	228.37	J/mol×K	441.34	Joback Method
cpg	217.38	J/mol×K	414.08	Joback Method

cpg	206.00	J/mol×K	386.82	Joback Method
dvisc	0.0006383	Pa×s	264.11	Joback Method
dvisc	0.0002409	Pa×s	359.56	Joback Method
dvisc	0.0003129	Pa×s	327.74	Joback Method
dvisc	0.0004301	Pa×s	295.92	Joback Method
dvisc	0.0050984	Pa×s	168.65	Joback Method
dvisc	0.0010554	Pa×s	232.29	Joback Method
dvisc	0.0020471	Pa×s	200.47	Joback Method
hvapt	35.80	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects

Sources

Cheméo Relay (1.0, beta):

Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects:	https://www.doi.org/10.1021/je800091s
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33838527&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume