8-methylpentadecane

Other names: Pentadecane, 8-methyl
Inchi: InChI=1S/C16H34/c1-4-6-8-10-12-14-16(3)15-13-11-9-7-5-2/h16H,4-15H2,1-3H3
InchiKey: OUKHTAOLUYDJTA-UHFFFAOYSA-N
Formula: C16H34
SMILES: CCCCCCCC(C)CCCCCCC
Mol. weight [g/mol]: 226.44
CAS: 22306-28-1

Physical Properties

Property code	Value	Unit	Source
af	0.6753		Cheméo Relay (1.0)
gf	81.40	kJ/mol	Joback Method
hf	-381.33	kJ/mol	Cheméo Relay (1.0)
hfus	33.67	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Cheméo Relay (1.0)
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-7.48		Cheméo Relay (1.0)
logp	6.344		Crippen Method
mcvol	236.300	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
tb	540.23	K	Cheméo Relay (1.0)
tc	699.17	K	Cheméo Relay (1.0)
tf	243.90 ± 2.00	K	NIST Webbook
vc	0.920	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.96	J/mol×K	565.04	Joback Method
cpg	631.47	J/mol×K	591.91	Joback Method
cpg	650.21	J/mol×K	618.79	Joback Method
cpg	668.20	J/mol×K	645.66	Joback Method
cpg	685.47	J/mol×K	672.53	Joback Method
cpg	702.03	J/mol×K	699.40	Joback Method

cpg	717.90	J/mol×K	726.28	Joback Method
dvisc	0.0077044	Pa×s	255.08	Joback Method
dvisc	0.0022640	Pa×s	306.74	Joback Method
dvisc	0.0009470	Pa×s	358.40	Joback Method
dvisc	0.0004934	Pa×s	410.06	Joback Method
dvisc	0.0002974	Pa×s	461.72	Joback Method
dvisc	0.0001985	Pa×s	513.38	Joback Method
dvisc	0.0001427	Pa×s	565.04	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
KDB:	https://www.cheric.org/files/research/kdb/mol/mol179.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22306281&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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