Cyclopentane, hexadecyl-

Other names: HEXADECYLCYCLOPENTANE
n-Hexadecylcyclopentane
Inchi: InChI=1S/C21H42/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-19-16-17-20-21/h21H,2-
InchiKey: YUMSFAHUVUYTKV-UHFFFAOYSA-N
Formula: C21H42
SMILES: CCCCCCCCCCCCCCCCC1CCCC1
Mol. weight [g/mol]: 294.56
CAS: 6812-39-1

Physical Properties

Property code	Value	Unit	Source
chl	-13850.80 ± 3.30	kJ/mol	NIST Webbook
gf	162.49	kJ/mol	Joback Method
hf	-415.60 ± 3.60	kJ/mol	NIST Webbook
hfus	44.08	kJ/mol	Joback Method
hvap	105.30	kJ/mol	NIST Webbook
log10ws	-8.27		Crippen Method
logp	8.048		Crippen Method
mcvol	295.890	ml/mol	McGowan Method
pc	1072.17	kPa	Joback Method
rinpol	2167.40		NIST Webbook
rinpol	2175.90		NIST Webbook
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
ripol	2184.40		NIST Webbook
tb	695.16	K	Joback Method
tc	869.82	K	Joback Method
tf	292.70 ± 1.00	K	NIST Webbook
tf	292.70 ± 1.00	K	NIST Webbook
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1016.86	J/mol×K	869.82	Joback Method
cpg	895.70	J/mol×K	695.16	Joback Method
cpg	918.47	J/mol×K	724.27	Joback Method
cpg	940.16	J/mol×K	753.38	Joback Method
cpg	960.80	J/mol×K	782.49	Joback Method
cpg	980.44	J/mol×K	811.60	Joback Method
cpg	999.11	J/mol×K	840.71	Joback Method
dvisc	0.0001236	Pa×s	695.16	Joback Method
dvisc	0.0035403	Pa×s	337.33	Joback Method
dvisc	0.0013297	Pa×s	396.97	Joback Method
dvisc	0.0006450	Pa×s	456.61	Joback Method
dvisc	0.0003698	Pa×s	516.25	Joback Method
dvisc	0.0002379	Pa×s	575.88	Joback Method
dvisc	0.0001663	Pa×s	635.52	Joback Method
hvapt	79.20	kJ/mol	586.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol606.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6812391&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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