Cyclooctadecanone

Inchi: InChI=1S/C18H34O/c19-18-16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-17-18/h1-17H2
InchiKey: WXAYGJXNCLBUDJ-UHFFFAOYSA-N
Formula: C18H34O
SMILES: O=C1CCCCCCCCCCCCCCCCC1
Mol. weight [g/mol]: 266.46
CAS: 6907-37-5

Physical Properties

Property code	Value	Unit	Source
gf	-134.95	kJ/mol	Joback Method
hf	-551.81	kJ/mol	Joback Method
hfus	7.45	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	6.201		Crippen Method
mcvol	255.190	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
tb	754.52	K	Joback Method
tc	1025.03	K	Joback Method
tf	330.22	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.37	J/mol×K	979.95	Joback Method
cpg	816.38	J/mol×K	754.52	Joback Method
cpg	848.30	J/mol×K	799.61	Joback Method
cpg	876.79	J/mol×K	844.69	Joback Method
cpg	901.72	J/mol×K	889.78	Joback Method
cpg	922.95	J/mol×K	934.86	Joback Method
cpg	953.85	J/mol×K	1025.03	Joback Method
hsubt	77.40 ± 0.80	kJ/mol	341.00	NIST Webbook
hvapt	64.00 ± 1.00	kJ/mol	353.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6907375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume