Cyclohexadecanone

Inchi: InChI=1S/C16H30O/c17-16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-16/h1-15H2
InchiKey: LXJDKGYSHYYKFJ-UHFFFAOYSA-N
Formula: C16H30O
SMILES: O=C1CCCCCCCCCCCCCCC1
Mol. weight [g/mol]: 238.41
CAS: 2550-52-9

Physical Properties

Property code	Value	Unit	Source
gf	-127.59	kJ/mol	Joback Method
hf	-498.21	kJ/mol	Joback Method
hfus	6.47	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.421		Crippen Method
mcvol	227.010	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2392.00		NIST Webbook
tb	700.22	K	Joback Method
tc	966.71	K	Joback Method
tf	314.72	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.22	J/mol×K	700.22	Joback Method
cpg	717.55	J/mol×K	744.64	Joback Method
cpg	746.07	J/mol×K	789.05	Joback Method
cpg	771.69	J/mol×K	833.47	Joback Method
cpg	794.30	J/mol×K	877.88	Joback Method

cpg	813.80	J/mol×K	922.30	Joback Method
cpg	830.08	J/mol×K	966.71	Joback Method
hsubt	82.00 ± 0.80	kJ/mol	333.00	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=C2550529&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
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