Cycloheptadecanone

Other names: Civetone, dihydro-
Dihydrocivetone
Inchi: InChI=1S/C17H32O/c18-17-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16-17/h1-16H2
InchiKey: KBQDZEMXPBDNGH-UHFFFAOYSA-N
Formula: C17H32O
SMILES: O=C1CCCCCCCCCCCCCCCC1
Mol. weight [g/mol]: 252.44
CAS: 3661-77-6

Physical Properties

Property code	Value	Unit	Source
gf	-131.27	kJ/mol	Joback Method
hf	-525.01	kJ/mol	Joback Method
hfus	6.96	kJ/mol	Joback Method
hvap	60.31	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.811		Crippen Method
mcvol	241.100	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
tb	727.37	K	Joback Method
tc	995.97	K	Joback Method
tf	322.47	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.62	J/mol×K	727.37	Joback Method
cpg	782.40	J/mol×K	772.14	Joback Method
cpg	811.07	J/mol×K	816.90	Joback Method
cpg	836.50	J/mol×K	861.67	Joback Method
cpg	858.60	J/mol×K	906.44	Joback Method
cpg	877.24	J/mol×K	951.21	Joback Method
cpg	892.31	J/mol×K	995.97	Joback Method

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=C3661776&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume