

Cyclotetradecanone-

Other names:	cyclotetradecan-1-one
Inchi:	InChI=1S/C14H26O/c15-14-12-10-8-6-4-2-1-3-5-7-9-11-13-14/h1-13H2
InchiKey:	FUGDHQXYVPQGLJ-UHFFFAOYSA-N
Formula:	C14H26O
SMILES:	O=C1CCCCCCCCCCCCC1
Mol. weight [g/mol]:	210.36
CAS:	3603-99-4

Physical Properties

Property code	Value	Unit	Source
gf	-120.23	kJ/mol	Joback Method
hf	-444.61	kJ/mol	Joback Method
hfus	5.49	kJ/mol	Joback Method
hvap	53.12	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.640		Crippen Method
mcvol	198.830	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
tb	645.92	K	Joback Method
tc	907.49	K	Joback Method
tf	299.22	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.37	J/mol×K	645.92	Joback Method
cpg	591.96	J/mol×K	689.51	Joback Method
cpg	619.31	J/mol×K	733.11	Joback Method
cpg	644.35	J/mol×K	776.70	Joback Method
cpg	666.99	J/mol×K	820.30	Joback Method
cpg	687.17	J/mol×K	863.89	Joback Method
cpg	704.79	J/mol×K	907.49	Joback Method
hsubt	80.80 ± 0.80	kJ/mol	310.00	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=C3603994&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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