

Oxacyclohexadecan-2-one, 16-methyl-

Other names:	15-Hexadecanolide (+/-)-15-Hexadecanolide (+/-)-15-hexadecanolide
Inchi:	InChI=1S/C16H30O2/c1-15-13-11-9-7-5-3-2-4-6-8-10-12-14-16(17)18-15/h15H,2-14H2,1
InchiKey:	GILZFLFJYUGJLX-UHFFFAOYSA-N
Formula:	C16H30O2
SMILES:	CC1CCCCCCCCCCCCC(=O)O1
Mol. weight [g/mol]:	254.41
CAS:	4459-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-221.42	kJ/mol	Joback Method
hf	-650.55	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.003		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
ripol	1959.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2304.00		NIST Webbook
ripol	2260.00		NIST Webbook
tb	722.50	K	Joback Method
tc	984.52	K	Joback Method
tf	337.05	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.50	J/mol×K	722.50	Joback Method
cpg	756.49	J/mol×K	766.17	Joback Method
cpg	783.67	J/mol×K	809.84	Joback Method
cpg	807.91	J/mol×K	853.51	Joback Method
cpg	829.10	J/mol×K	897.18	Joback Method
cpg	847.13	J/mol×K	940.85	Joback Method
cpg	861.88	J/mol×K	984.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4459578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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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