

Oxacyclotetradecan-2-one, 14-methyl-

Other names:	13-Tetradecanolide
Inchi:	InChI=1S/C14H26O2/c1-13-11-9-7-5-3-2-4-6-8-10-12-14(15)16-13/h13H,2-12H2,1H3
InchiKey:	FGDBANZBXSCEG-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CC1CCCCCCCCCCCCC(=O)O1
Mol. weight [g/mol]:	226.35
CAS:	27198-63-6

Physical Properties

Property code	Value	Unit	Source
gf	-214.06	kJ/mol	Joback Method
hf	-596.95	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	57.32	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.223		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2057.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2056.00		NIST Webbook
tb	668.20	K	Joback Method
tc	925.56	K	Joback Method
tf	321.55	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	601.26	J/mol×K	668.20	Joback Method
cpg	629.85	J/mol×K	711.09	Joback Method
cpg	656.21	J/mol×K	753.99	Joback Method
cpg	680.23	J/mol×K	796.88	Joback Method
cpg	701.84	J/mol×K	839.77	Joback Method
cpg	720.93	J/mol×K	882.67	Joback Method
cpg	737.41	J/mol×K	925.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27198636&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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