

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]:	226.36

Physical Properties

Property code	Value	Unit	Source
hf	-636.67	kJ/mol	Cheméo Relay (1.0)
hfus	14.54	kJ/mol	Joback Method
hvap	78.18	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	-3.70		Cheméo Relay (1.0)
logp	4.223		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2057.00		NIST Webbook
ripol	2056.00		NIST Webbook
tb	633.41	K	Cheméo Relay (1.0)
tf	308.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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