

Oxa-2-cyclotetradecanone

Inchi:	InChI=1S/C17H32O2/c18-17-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16-19-17/h1-16H2
InchiKey:	FXQOOHFUXNQCKQ-UHFFFAOYSA-N
Formula:	C17H32O2
SMILES:	O=C1CCCCCCCCCCCCCCCCO1
Mol. weight [g/mol]:	268.43
CAS:	5637-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-229.49	kJ/mol	Joback Method
hf	-663.17	kJ/mol	Joback Method
hfus	12.84	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.395		Crippen Method
mcvol	246.970	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2042.30		NIST Webbook
rinpol	2051.00		NIST Webbook
rinpol	2042.30		NIST Webbook
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook
ripol	2433.00		NIST Webbook
ripol	2433.00		NIST Webbook
tb	758.59	K	Joback Method
tc	1030.72	K	Joback Method
tf	345.52	K	Joback Method
vc	0.854	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.60	J/mol×K	758.59	Joback Method

cpg	824.08	J/mol×K	803.95	Joback Method
cpg	851.15	J/mol×K	849.30	Joback Method
cpg	874.67	J/mol×K	894.66	Joback Method
cpg	894.49	J/mol×K	940.01	Joback Method
cpg	910.47	J/mol×K	985.37	Joback Method
cpg	922.48	J/mol×K	1030.72	Joback Method
hvapt	73.50	kJ/mol	433.00	NIST Webbook

Sources

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=C5637978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
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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