

Cyclocoloronone

Other names:	Cyclocorolonone
Inchi:	InChI=1S/C15H22O/c1-8-5-6-11-14(15(11,3)4)13-9(2)12(16)7-10(8)13/h8,10-11,14H,5-7
InchiKey:	ZEEUIOBUKGZKPS-ZOAVQCKWSA-N
Formula:	C15H22O
SMILES:	<chem>CC1=C2C(CC1=O)C(C)CCC1C2C1(C)C</chem>
Mol. weight [g/mol]:	218.33
CAS:	489-45-2

Physical Properties

Property code	Value	Unit	Source
gf	100.67	kJ/mol	Joback Method
hf	-275.15	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	53.16	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1788.00		NIST Webbook
ripol	2254.00		NIST Webbook
tb	639.20	K	Joback Method
tc	869.72	K	Joback Method
tf	415.03	K	Joback Method
vc	0.720	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.90	J/molxK	639.20	Joback Method
cpg	567.48	J/molxK	677.62	Joback Method
cpg	587.88	J/molxK	716.04	Joback Method
cpg	607.27	J/molxK	754.46	Joback Method
cpg	625.82	J/molxK	792.88	Joback Method
cpg	643.70	J/molxK	831.30	Joback Method
cpg	661.06	J/molxK	869.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C489452&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

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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