

Cyperenal

Inchi:	InChI=1S/C14H20O/c1-13(2)11-4-3-6-14(13)7-5-10(9-15)12(14)8-11/h9,11H,3-8H2,1-2H
InchiKey:	JMTHIKZIQLFHDG-FZMZJTMJSA-N
Formula:	C14H20O
SMILES:	CC1(C)C2CCCC13CCC(C=O)=C3C2
Mol. weight [g/mol]:	204.31

Physical Properties

Property code	Value	Unit	Source
gf	125.25	kJ/mol	Joback Method
hf	-146.47	kJ/mol	Joback Method
hfus	12.36	kJ/mol	Joback Method
hvap	52.88	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.492		Crippen Method
mvol	172.810	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
tb	606.74	K	Joback Method
tc	839.85	K	Joback Method
tf	409.92	K	Joback Method
vc	0.673	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.08	J/mol×K	606.74	Joback Method
cpg	494.82	J/mol×K	645.59	Joback Method
cpg	512.38	J/mol×K	684.44	Joback Method
cpg	529.08	J/mol×K	723.30	Joback Method
cpg	545.25	J/mol×K	762.15	Joback Method
cpg	561.24	J/mol×K	801.00	Joback Method
cpg	577.36	J/mol×K	839.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R334275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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