

9-Cedranone

Other names:	5-Cedranone
Inchi:	InChI=1S/C15H24O/c1-9-5-6-13-14(3,4)11-7-15(9,13)8-12(16)10(11)2/h9-11,13H,5-8H2,
InchiKey:	CHPQWDBBFXQHQC-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1C(=O)CC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	76.77	kJ/mol	Joback Method
hf	-315.09	kJ/mol	Joback Method
hfus	14.94	kJ/mol	Joback Method
hvap	50.08	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.674		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1638.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1599.00		NIST Webbook
tb	625.65	K	Joback Method
tc	861.18	K	Joback Method
tf	408.89	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.07	J/molxK	625.65	Joback Method
cpg	589.71	J/molxK	664.90	Joback Method
cpg	612.09	J/molxK	704.16	Joback Method
cpg	633.49	J/molxK	743.41	Joback Method
cpg	654.20	J/molxK	782.67	Joback Method

cpg	674.52	J/mol×K	821.92	Joback Method
cpg	694.73	J/mol×K	861.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U156232&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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