

Cedranone

Other names:	Cedranone 5 8bH-Cedran-9-one
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
CAS:	13567-40-3

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	1600.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1617.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	2030.00		NIST Webbook
tb	625.65	K	Joback Method
tc	861.18	K	Joback Method
tf	408.89	K	Joback Method
vc	0.731	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13567403&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

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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