

Calamenone

Inchi:	InChI=1S/C14H22O2/c1-8-4-5-10-13(2,3)12(16)9-6-11(15)14(8,10)7-9/h8-11,15H,4-7H2,
InchiKey:	ZPXYQKMXCQAADS-BYYFJZQESA-N
Formula:	C14H22O2
SMILES:	CC1CCC2C(C)(C)C(=O)C3CC(O)C12C3
Mol. weight [g/mol]:	222.32

Physical Properties

Property code	Value	Unit	Source
gf	-68.47	kJ/mol	Joback Method
hf	-446.68	kJ/mol	Joback Method
hfus	16.44	kJ/mol	Joback Method
hvap	64.54	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.399		Crippen Method
mcvol	182.980	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1685.00		NIST Webbook
tb	694.95	K	Joback Method
tc	915.65	K	Joback Method
tf	458.44	K	Joback Method
vc	0.694	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.62	J/mol×K	694.95	Joback Method
cpg	600.78	J/mol×K	731.73	Joback Method
cpg	619.32	J/mol×K	768.52	Joback Method
cpg	637.47	J/mol×K	805.30	Joback Method
cpg	655.47	J/mol×K	842.09	Joback Method
cpg	673.57	J/mol×K	878.87	Joback Method
cpg	692.00	J/mol×K	915.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R231666&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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