Capnellane-8-one

Inchi: InChI=1S/C15H24O/c1-9-11(16)7-10-8-15(4)6-5-14(2,3)13(15)12(9)10/h9-10,12-13H,5-8
InchiKey: OUWRASYSJBAWAF-OLAWPIOWSA-N
Formula: C15H24O
SMILES: CC1C(=O)CC2CC3(C)CCC(C)(C)C3C21
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	1942.00		NIST Webbook
rinpol	1942.00		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/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

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=R287426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume