10-Nor-calamenen-10-one

Inchi: InChI=1S/C14H18O/c1-9(2)11-6-7-14(15)12-5-4-10(3)8-13(11)12/h4-5,8-9,11H,6-7H2,1-
InchiKey: KIZXBPVAPQXAMH-UHFFFAOYSA-N
Formula: C14H18O
SMILES: Cc1ccc2c(c1)C(C(C)C)CCC2=O
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	83.77	kJ/mol	Joback Method
hf	-195.04	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	54.30	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.711		Crippen Method
mcvol	175.070	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1707.00		NIST Webbook
tb	634.75	K	Joback Method
tc	870.27	K	Joback Method
tf	366.64	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.33	J/mol×K	634.75	Joback Method
cpg	484.30	J/mol×K	674.00	Joback Method
cpg	502.07	J/mol×K	713.26	Joback Method
cpg	518.66	J/mol×K	752.51	Joback Method
cpg	534.11	J/mol×K	791.77	Joback Method
cpg	548.44	J/mol×K	831.02	Joback Method

cpg	561.69	J/mol×K	870.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R610678&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
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