«alpha»-Longipinen-2-one (Vulgarone B)

Inchi: InChI=1S/C15H22O/c1-9-8-10(16)12-13-11(9)15(12,4)7-5-6-14(13,2)3/h8,11-13H,5-7H2,
InchiKey: KTPOZFYJWLGJGH-HJZMNPPUSA-N
Formula: C15H22O
SMILES: CC1=CC(=O)C2C3C1C2(C)CCCC3(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	104.81	kJ/mol	Joback Method
hf	-248.44	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1596.00		NIST Webbook
tb	634.46	K	Joback Method
tc	873.09	K	Joback Method
tf	426.41	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.90	J/mol×K	634.46	Joback Method
cpg	564.64	J/mol×K	674.23	Joback Method
cpg	585.28	J/mol×K	714.00	Joback Method
cpg	605.11	J/mol×K	753.77	Joback Method
cpg	624.46	J/mol×K	793.54	Joback Method
cpg	643.61	J/mol×K	833.32	Joback Method

cpg	662.89	J/mol×K	873.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R226609&Units=SI
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

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