Longiverbenone

Other names: Vulgarone B
Longiverbenone (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-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC1=CC(=O)C2C3C1C2(C)CCCC3(C)C
Mol. weight [g/mol]: 218.33
CAS: 64180-68-3

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	1675.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1658.20		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1658.20		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1632.00		NIST Webbook

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rinpol	1627.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1651.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2254.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2265.00		NIST Webbook
ripol	2265.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2254.00		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

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=C64180683&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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