

Longipinanol

Other names:	trans-longipinanol
Inchi:	InChI=1S/C15H26O/c1-13(2)7-5-8-14(3)10-6-9-15(4,16)12(14)11(10)13/h10-12,16H,5-9H
InchiKey:	QDCXLQJUFNZYHG-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC1(C)CCCC2(C)C3CCC(C)(O)C2C31
Mol. weight [g/mol]:	222.37
CAS:	39703-23-6

Physical Properties

Property code	Value	Unit	Source
gf	57.05	kJ/mol	Joback Method
hf	-314.38	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.610		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1567.00		NIST Webbook
ripol	1985.00		NIST Webbook
ripol	1985.00		NIST Webbook
tb	650.25	K	Joback Method
tc	863.66	K	Joback Method
tf	425.39	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.75	J/mol×K	650.25	Joback Method
cpg	615.74	J/mol×K	685.82	Joback Method
cpg	634.97	J/mol×K	721.39	Joback Method
cpg	653.76	J/mol×K	756.96	Joback Method
cpg	672.45	J/mol×K	792.52	Joback Method
cpg	691.37	J/mol×K	828.09	Joback Method
cpg	710.84	J/mol×K	863.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C39703236&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

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