epi-Longipinanol

Inchi: InChI=1S/C15H26O/c1-9-10-6-8-15(4,16)13-11(9)5-7-14(2,3)12(10)13/h9-13,16H,5-8H2,
InchiKey: WHIUDXGNUHDGLA-RTSMVLBVSA-N
Formula: C15H26O
SMILES: CC1C2CCC(C)(O)C3C1CCC(C)(C)C23
Mol. weight [g/mol]: 222.37
CAS: 54275-23-9

Physical Properties

Property code	Value	Unit	Source
gf	54.83	kJ/mol	Joback Method
hf	-349.96	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.466		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	645.34	K	Joback Method
tc	851.43	K	Joback Method
tf	397.25	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.58	J/mol×K	645.34	Joback Method

cpg	621.09	J/mol×K	679.69	Joback Method
cpg	640.66	J/mol×K	714.04	Joback Method
cpg	659.50	J/mol×K	748.38	Joback Method
cpg	677.83	J/mol×K	782.73	Joback Method
cpg	695.86	J/mol×K	817.08	Joback Method
cpg	713.82	J/mol×K	851.43	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=C54275239&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