

Himachalenol

Inchi: InChI=1S/C15H24O/c1-11-6-7-13-12(2)5-4-8-15(3,10-16)14(13)9-11/h9,14,16H,4-8,10H2
InchiKey: WQWZZNAYNUIRFF-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1=CC2C(=C(C)CCCC2(C)CO)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	25.14	kJ/mol	Joback Method
hf	-293.97	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	67.77	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.842		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1637.00		NIST Webbook
ripol	2108.00		NIST Webbook
tb	683.11	K	Joback Method
tc	894.07	K	Joback Method
tf	400.89	K	Joback Method
vc	0.739	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.59	J/mol×K	683.11	Joback Method
cpg	590.84	J/mol×K	718.27	Joback Method
cpg	608.22	J/mol×K	753.43	Joback Method
cpg	624.85	J/mol×K	788.59	Joback Method
cpg	640.86	J/mol×K	823.75	Joback Method
cpg	656.35	J/mol×K	858.91	Joback Method
cpg	671.46	J/mol×K	894.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R516328&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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