

«beta»-HIMACHALENOXIDE

Other names:	«beta»-Himachalene oxide «beta»-Himachalene epoxide
Inchi:	InChI=1S/C15H24O/c1-10-6-5-8-14(2,3)12-11(10)7-9-15(4)13(12)16-15/h12-13H,5-9H2,
InchiKey:	GUMYGCGJGNRHGS-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1=C2CCC3(C)OC3C2C(C)(C)CCC1
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	127.26	kJ/mol	Joback Method
hf	-240.03	kJ/mol	Joback Method
hfus	19.61	kJ/mol	Joback Method
hvap	52.75	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.080		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1612.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1612.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2045.00		NIST Webbook
tb	607.51	K	Joback Method
tc	839.29	K	Joback Method
tf	398.00	K	Joback Method
vc	0.725	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	539.97	J/mol×K	607.51	Joback Method
cpg	561.95	J/mol×K	646.14	Joback Method
cpg	582.62	J/mol×K	684.77	Joback Method
cpg	602.29	J/mol×K	723.40	Joback Method
cpg	621.26	J/mol×K	762.03	Joback Method
cpg	639.84	J/mol×K	800.66	Joback Method
cpg	658.34	J/mol×K	839.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U140216&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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