

himachalene oxide

Other names:

himachalene epoxide

(4aS)-3,5,5,9-Tetramethyl-1,2,5,6,7,8-hexahydro-4a,8-epoxybenzo[7]annulene

Inchi:

InChI=1S/C15H22O/c1-10-5-6-12-11(2)13-7-8-14(3,4)15(12,9-10)16-13/h9,13H,5-8H2,1-

InchiKey:

HBZPFOFGXNILSW-UHFFFAOYSA-N

Formula:

C15H22O

SMILES:CC1=CC23OC(CCC2(C)C)C(C)=C3CC1**Mol. weight [g/mol]:**

218.33

CAS:

64825-84-9

Physical Properties

Property code	Value	Unit	Source
gf	155.30	kJ/mol	Joback Method
hf	-173.38	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	54.02	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.001		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1584.40		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1584.40		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	616.32	K	Joback Method
tc	851.24	K	Joback Method
tf	415.52	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.41	J/mol×K	616.32	Joback Method
cpg	537.44	J/mol×K	655.47	Joback Method
cpg	556.31	J/mol×K	694.63	Joback Method
cpg	574.36	J/mol×K	733.78	Joback Method
cpg	591.90	J/mol×K	772.93	Joback Method
cpg	609.25	J/mol×K	812.09	Joback Method
cpg	626.75	J/mol×K	851.24	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=C64825849&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
mccvol:	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

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