

«beta»-Cedrene epoxide

Inchi: InChI=1S/C15H24O/c1-10-4-5-11-13(2,3)12-8-14(10,11)6-7-15(12)9-16-15/h10-12H,4-9H
InchiKey: BWDPPCMUUFETAC-MJAQFUTBSA-N
Formula: C15H24O
SMILES: CC1CCC2C(C)(C)C3CC12CCC31CO1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	188.31	kJ/mol	Joback Method
hf	-194.85	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	49.25	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.628		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1596.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2046.00		NIST Webbook
tb	592.16	K	Joback Method
tc	829.78	K	Joback Method
tf	416.84	K	Joback Method
vc	0.709	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	541.84	J/mol×K	592.16	Joback Method
cpg	564.86	J/mol×K	631.76	Joback Method
cpg	586.26	J/mol×K	671.37	Joback Method
cpg	606.55	J/mol×K	710.97	Joback Method
cpg	626.24	J/mol×K	750.57	Joback Method
cpg	645.84	J/mol×K	790.17	Joback Method
cpg	665.85	J/mol×K	829.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R397716&Units=SI
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

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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