

Cabreuva oxide B

Inchi:

InChI=1S/C15H24O/c1-6-15(5)10-12-9-11(2)7-8-13(12)14(3,4)16-15/h6,9,12-13H,1,7-8,1

InchiKey:

NIGRJVWIKNICMW-YDHLFZDLSA-N

Formula:

C15H24O

SMILES:

C=CC1(C)CC2C=C(C)CCC2C(C)(C)O1

Mol. weight [g/mol]:

220.35

Physical Properties

Property code	Value	Unit	Source
gf	144.17	kJ/mol	Joback Method
hf	-202.43	kJ/mol	Joback Method
hfus	19.55	kJ/mol	Joback Method
hvap	51.37	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.103		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
ripol	1712.00		NIST Webbook
tb	592.07	K	Joback Method
tc	819.27	K	Joback Method
tf	358.02	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.65	J/mol×K	592.07	Joback Method
cpg	557.08	J/mol×K	629.94	Joback Method
cpg	578.17	J/mol×K	667.80	Joback Method

cpg	598.16	J/mol×K	705.67	Joback Method
cpg	617.32	J/mol×K	743.54	Joback Method
cpg	635.90	J/mol×K	781.40	Joback Method
cpg	654.14	J/mol×K	819.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232565&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
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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