Cabreuva oxide-VI

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-UHFFFAOYSA-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
ripol	1823.00		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=R328240&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume