Cadinan-10-«beta»-ol, 2-«alpha»,3-«alpha»-epoxy

Inchi: InChI=1S/C15H26O2/c1-8(2)10-5-6-15(4,16)12-11(10)7-9(3)13-14(12)17-13/h8-14,16H,5

InchiKey: RSTBBOJWVDGMGG-CRIWNQTOSA-N

Formula: C15H26O2

SMILES: CC(C)C1CCC(C)(O)C2C1CC(C)C1OC12

Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-28.24	kJ/mol	Joback Method
hf	-502.48	kJ/mol	Joback Method
hfus	31.34	kJ/mol	Joback Method
hvap	67.48	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.843		Crippen Method
mcvol	201.370	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1760.00		NIST Webbook
tb	671.61	K	Joback Method
tc	873.23	K	Joback Method
tf	384.92	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.90	J/mol×K	671.61	Joback Method
cpg	659.99	J/mol×K	705.21	Joback Method
cpg	679.10	J/mol×K	738.82	Joback Method
cpg	697.34	J/mol×K	772.42	Joback Method
cpg	714.86	J/mol×K	806.03	Joback Method
cpg	731.80	J/mol×K	839.63	Joback Method
cpg	748.27	J/mol×K	873.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R391510&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume