3,15-«beta»-Epoxy-4«beta»-acetoxygymnomitrane

Other names: (-)3«beta»,15«beta»-Epoxy-4«beta»-acetoxygymnomitrane
Inchi: InChI=1S/C17H26O3/c1-11(18)20-13-9-14(2)8-12(17(13)10-19-17)15(3)6-5-7-16(14,15)4
InchiKey: RPIPUNFNXUXZEF-FAZLRTIUSA-N
Formula: C17H26O3
SMILES: CC(=O)OC1CC2(C)CC(C13CO3)C1(C)CCCC21C
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-34.26	kJ/mol	Joback Method
hf	-465.69	kJ/mol	Joback Method
hfus	17.94	kJ/mol	Joback Method
hvap	61.70	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.313		Crippen Method
mcvol	220.260	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
tb	714.45	K	Joback Method
tc	953.81	K	Joback Method
tf	535.44	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.38	J/mol×K	714.45	Joback Method
cpg	723.44	J/mol×K	754.34	Joback Method
cpg	745.69	J/mol×K	794.24	Joback Method
cpg	768.74	J/mol×K	834.13	Joback Method
cpg	793.21	J/mol×K	874.02	Joback Method
cpg	819.72	J/mol×K	913.91	Joback Method
cpg	848.88	J/mol×K	953.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R425648&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume