epi-Me-dihydrophaseic acid

Inchi: InChI=1S/C15H22O5/c1-10(6-12(17)18)4-5-15(19)13(2)7-11(16)8-14(15,3)20-9-13/h4-6,
InchiKey: XIVFQYWMMJWUCD-MIYZNNEXSA-N
Formula: C15H22O5
SMILES: CC(C=CC1(O)C2(C)COC1(C)CC(O)C2)=CC(=O)O
Mol. weight [g/mol]: 282.33

Physical Properties

Property code	Value	Unit	Source
gf	-332.78	kJ/mol	Joback Method
hf	-691.23	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	106.37	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.254		Crippen Method
mcvol	216.940	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	921.56	K	Joback Method
tc	1134.10	K	Joback Method
tf	585.71	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.44	J/mol×K	921.56	Joback Method
cpg	766.52	J/mol×K	956.98	Joback Method
cpg	789.46	J/mol×K	992.41	Joback Method
cpg	814.59	J/mol×K	1027.83	Joback Method
cpg	842.23	J/mol×K	1063.25	Joback Method
cpg	872.74	J/mol×K	1098.67	Joback Method
cpg	906.43	J/mol×K	1134.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R487364&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