epi-Me-dihydrophaseic acid-Ac

Inchi: InChI=1S/C18H26O6/c1-12(8-15(20)22-5)6-7-18(21)16(3)9-14(24-13(2)19)10-17(18,4)23
InchiKey: ONGJVIGGHJEDKU-IWPPBABSSA-N
Formula: C18H26O6
SMILES: COC(=O)C=C(C)C=CC1(O)C2(C)COC1(C)CC(OC(C)=O)C2
Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-372.80	kJ/mol	Joback Method
hf	-825.71	kJ/mol	Joback Method
hfus	34.43	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	1.914		Crippen Method
mcvol	260.780	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	2247.00		NIST Webbook
tb	904.55	K	Joback Method
tc	1125.11	K	Joback Method
tf	592.27	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.85	J/mol×K	904.55	Joback Method
cpg	898.01	J/mol×K	941.31	Joback Method
cpg	922.61	J/mol×K	978.07	Joback Method
cpg	948.97	J/mol×K	1014.83	Joback Method
cpg	977.45	J/mol×K	1051.59	Joback Method
cpg	1008.38	J/mol×K	1088.35	Joback Method
cpg	1042.12	J/mol×K	1125.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R487379&Units=SI

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