Me-2-trans-dihydrophaseic acid

Inchi: InChI=1S/C16H24O5/c1-11(7-13(18)20-4)5-6-16(19)14(2)8-12(17)9-15(16,3)21-10-14/h5
InchiKey: QNMHUZMKLBWTQM-PSCDLIPDSA-N
Formula: C16H24O5
SMILES: COC(=O)C=C(C)C=CC1(O)C2(C)COC1(C)CC(O)C2
Mol. weight [g/mol]: 296.36

Physical Properties

Property code	Value	Unit	Source
gf	-292.54	kJ/mol	Joback Method
hf	-691.86	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.343		Crippen Method
mcvol	231.030	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook
tb	874.68	K	Joback Method
tc	1086.40	K	Joback Method
tf	558.39	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.50	J/mol×K	874.68	Joback Method
cpg	788.53	J/mol×K	909.97	Joback Method
cpg	809.81	J/mol×K	945.25	Joback Method
cpg	832.67	J/mol×K	980.54	Joback Method
cpg	857.42	J/mol×K	1015.82	Joback Method
cpg	884.38	J/mol×K	1051.11	Joback Method
cpg	913.86	J/mol×K	1086.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R487408&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