Methyldavanate

Inchi: InChI=1S/C16H24O4/c1-6-16(4)10-9-14(20-16)12(3)13(17)8-7-11(2)15(18)19-5/h6-7,12,
InchiKey: ZWWRGHCKXZFVDX-WLWNCFMFSA-N
Formula: C16H24O4
SMILES: C=CC1(C)CCC(C(C)C(=O)CC=C(C)C(=O)OC)O1
Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-184.70	kJ/mol	Joback Method
hf	-579.99	kJ/mol	Joback Method
hfus	32.36	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.825		Crippen Method
mcvol	231.720	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1241.00		NIST Webbook
tb	733.72	K	Joback Method
tc	946.01	K	Joback Method
tf	413.50	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.42	J/mol×K	733.72	Joback Method
cpg	697.13	J/mol×K	769.10	Joback Method
cpg	714.05	J/mol×K	804.48	Joback Method
cpg	730.33	J/mol×K	839.86	Joback Method
cpg	746.09	J/mol×K	875.24	Joback Method
cpg	761.44	J/mol×K	910.63	Joback Method
cpg	776.52	J/mol×K	946.01	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=R229326&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