apodophyllone

Inchi: InChI=1S/C15H22O4/c1-8(2)12(16)11-14(18-6)9(3)13(17-5)10(4)15(11)19-7/h8H,1-7H3
InchiKey: XLMIFOSFHOIPHQ-UHFFFAOYSA-N
Formula: C15H22O4
SMILES: COc1c(C)c(OC)c(C(=O)C(C)C)c(OC)c1C
Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-306.68	kJ/mol	Joback Method
hf	-688.27	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	68.16	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.168		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1685.00		NIST Webbook
tb	714.87	K	Joback Method
tc	917.11	K	Joback Method
tf	449.45	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.13	J/mol×K	714.87	Joback Method
cpg	615.86	J/mol×K	748.58	Joback Method
cpg	630.73	J/mol×K	782.28	Joback Method
cpg	644.72	J/mol×K	815.99	Joback Method
cpg	657.81	J/mol×K	849.70	Joback Method
cpg	669.97	J/mol×K	883.40	Joback Method
cpg	681.18	J/mol×K	917.11	Joback Method
dvisc	0.0004461	Pa×s	449.45	Joback Method
dvisc	0.0002905	Pa×s	493.69	Joback Method

dvisc	0.0002031	Pa×s	537.92	Joback Method
dvisc	0.0001499	Pa×s	582.16	Joback Method
dvisc	0.0001155	Pa×s	626.40	Joback Method
dvisc	0.0000921	Pa×s	670.63	Joback Method
dvisc	0.0000755	Pa×s	714.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301765&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
dvisc:	Dynamic viscosity
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