2,3-Divanillyl-1,4-butanediol

Inchi: InChI=1S/C20H26O6/c1-25-19-9-13(3-5-17(19)23)7-15(11-21)16(12-22)8-14-4-6-18(24)2
InchiKey: PUETUDUXMCLALY-UHFFFAOYSA-N
Formula: C20H26O6
SMILES: COc1cc(CC(CO)C(CO)Cc2ccc(O)c(OC)c2)ccc1O
Mol. weight [g/mol]: 362.42
CAS: 3688-23-1

Physical Properties

Property code	Value	Unit	Source
gf	-474.68	kJ/mol	Joback Method
hf	-940.09	kJ/mol	Joback Method
hfus	49.93	kJ/mol	Joback Method
hvap	129.42	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.117		Crippen Method
mcvol	280.360	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinpol	3247.20		NIST Webbook
rinpol	3247.20		NIST Webbook
tb	1109.88	K	Joback Method
tc	1359.40	K	Joback Method
tf	752.58	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.88	J/mol×K	1109.88	Joback Method
cpg	1053.60	J/mol×K	1317.81	Joback Method
cpg	1036.06	J/mol×K	1276.23	Joback Method
cpg	1019.20	J/mol×K	1234.64	Joback Method
cpg	1002.83	J/mol×K	1193.05	Joback Method
cpg	986.78	J/mol×K	1151.47	Joback Method
cpg	1071.97	J/mol×K	1359.40	Joback Method

dvisc	4.3139424e-10	Pa×s	1109.88	Joback Method
dvisc	7.5446111e-10	Pa×s	1050.33	Joback Method
dvisc	1.4111769e-09	Pa×s	990.78	Joback Method
dvisc	2.8596079e-09	Pa×s	931.23	Joback Method
dvisc	6.3817562e-09	Pa×s	871.68	Joback Method
dvisc	1.6021440e-08	Pa×s	812.13	Joback Method
dvisc	4.6529390e-08	Pa×s	752.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3688231&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
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