Pyrogallol, isoBOC

Inchi: InChI=1S/C21H30O9/c1-13(2)10-25-19(22)28-16-8-7-9-17(29-20(23)26-11-14(3)4)18(16
InchiKey: IXJIOOQBENUBJB-UHFFFAOYSA-N
Formula: C21H30O9
SMILES: CC(C)COC(=O)Oc1cccc(OC(=O)OCC(C)C)c1OC(=O)OCC(C)C
Mol. weight [g/mol]: 426.46

Physical Properties

Property code	Value	Unit	Source
gf	-804.99	kJ/mol	Joback Method
hf	-1410.08	kJ/mol	Joback Method
hfus	44.76	kJ/mol	Joback Method
hvap	99.47	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.201		Crippen Method
mcvol	322.920	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2486.00		NIST Webbook
tb	1011.33	K	Joback Method
tc	1238.29	K	Joback Method
tf	616.06	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.33	J/mol×K	1011.33	Joback Method
cpg	1071.75	J/mol×K	1049.16	Joback Method
cpg	1080.01	J/mol×K	1086.98	Joback Method
cpg	1086.06	J/mol×K	1124.81	Joback Method
cpg	1089.87	J/mol×K	1162.64	Joback Method
cpg	1091.38	J/mol×K	1200.47	Joback Method
cpg	1090.54	J/mol×K	1238.29	Joback Method
dvisc	0.0001163	Pa×s	616.06	Joback Method
dvisc	0.0000641	Pa×s	681.94	Joback Method

dvisc	0.0000392	Pa×s	747.82	Joback Method
dvisc	0.0000260	Pa×s	813.69	Joback Method
dvisc	0.0000183	Pa×s	879.57	Joback Method
dvisc	0.0000135	Pa×s	945.45	Joback Method
dvisc	0.0000104	Pa×s	1011.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235351&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