Monotropitoside

Inchi: InChI=1S/C19H26O12/c1-27-17(26)8-4-2-3-5-10(8)30-19-16(25)14(23)13(22)11(31-19)7
InchiKey: VHUNCYDAXJGCLO-UHFFFAOYSA-N
Formula: C19H26O12
SMILES: COC(=O)c1ccccc1OC1OC(COC2OCC(O)C(O)C2O)C(O)C(O)C1O
Mol. weight [g/mol]: 446.40

Physical Properties

Property code	Value	Unit	Source
gf	-1230.27	kJ/mol	Joback Method
hf	-1930.79	kJ/mol	Joback Method
hfus	75.43	kJ/mol	Joback Method
hvap	182.59	kJ/mol	Joback Method
log10ws	-0.74		Estimated Solubility Method
log10ws	-0.74		Aqueous Solubility Prediction Method
logp	-2.885		Crippen Method
mcvol	299.230	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
tb	1400.30	K	Joback Method
tc	1902.63	K	Joback Method
tf	862.59	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.79	J/mol×K	1400.30	Joback Method
cpg	742.82	J/mol×K	1818.91	Joback Method
cpg	838.82	J/mol×K	1735.19	Joback Method
cpg	920.19	J/mol×K	1651.47	Joback Method
cpg	987.25	J/mol×K	1567.74	Joback Method
cpg	1040.34	J/mol×K	1484.02	Joback Method
cpg	631.84	J/mol×K	1902.63	Joback Method

dvisc	1.3277043e-10	Pa×s	1400.30	Joback Method
dvisc	2.3831620e-10	Pa×s	1310.68	Joback Method
dvisc	4.6611964e-10	Pa×s	1221.06	Joback Method
dvisc	1.0138978e-09	Pa×s	1131.44	Joback Method
dvisc	2.5208914e-09	Pa×s	1041.83	Joback Method
dvisc	7.4399738e-09	Pa×s	952.21	Joback Method
dvisc	2.7494958e-08	Pa×s	862.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume