2,3-dihydroxypropyl 2-(6-methoxynaphthalen-2-yl)propanoate

Inchi: InChI=1S/C17H20O5/c1-11(17(20)22-10-15(19)9-18)12-3-4-14-8-16(21-2)6-5-13(14)7-12

InchiKey: NQGWSPZQESAHBV-UHFFFAOYSA-N

Formula: C17H20O5

SMILES: COc1ccc2cc(C(C)C(=O)OCC(O)CO)ccc2c1

Mol. weight [g/mol]: 304.34

Physical Properties

Property code	Value	Unit	Source
gf	-325.38	kJ/mol	Joback Method
hf	-681.59	kJ/mol	Joback Method
hfus	35.17	kJ/mol	Joback Method
hvap	102.82	kJ/mol	Joback Method
log10ws	-2.62		Aqueous Solubility Prediction Method
logp	1.848		Crippen Method
mcvol	232.220	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
tb	926.17	K	Joback Method
tc	1138.50	K	Joback Method
tf	551.54	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.17	J/mol×K	926.17	Joback Method
cpg	734.81	J/mol×K	961.56	Joback Method
cpg	744.61	J/mol×K	996.95	Joback Method
cpg	753.62	J/mol×K	1032.34	Joback Method
cpg	761.86	J/mol×K	1067.72	Joback Method
cpg	769.38	J/mol×K	1103.11	Joback Method
cpg	776.22	J/mol×K	1138.50	Joback Method
dvisc	0.0001693	Pa×s	551.54	Joback Method
dvisc	0.0000609	Pa×s	613.98	Joback Method

dvisc	0.0000264	Pa×s	676.42	Joback Method
dvisc	0.0000132	Pa×s	738.86	Joback Method
dvisc	0.0000074	Pa×s	801.29	Joback Method
dvisc	0.0000045	Pa×s	863.73	Joback Method
dvisc	0.0000029	Pa×s	926.17	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

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