

2-hydroxyethyl 2-(6-methoxynaphthalen-2-yl)propanoate

Inchi:	InChI=1S/C16H18O4/c1-11(16(18)20-8-7-17)12-3-4-14-10-15(19-2)6-5-13(14)9-12/h3-6,
InchiKey:	NYYKRAQUHNVACN-UHFFFAOYSA-N
Formula:	C16H18O4
SMILES:	COc1ccc2cc(C(C)C(=O)OCCO)ccc2c1
Mol. weight [g/mol]:	274.32

Physical Properties

Property code	Value	Unit	Source
gf	-194.54	kJ/mol	Joback Method
hf	-503.44	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	84.31	kJ/mol	Joback Method
log10ws	-3.33		Aqueous Solubility Prediction Method
logp	2.487		Crippen Method
mcvol	212.260	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
tb	811.55	K	Joback Method
tc	1020.94	K	Joback Method
tf	494.45	K	Joback Method
vc	0.800	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.93	J/mol×K	811.55	Joback Method
cpg	630.23	J/mol×K	846.45	Joback Method
cpg	641.68	J/mol×K	881.35	Joback Method
cpg	652.30	J/mol×K	916.25	Joback Method
cpg	662.13	J/mol×K	951.15	Joback Method
cpg	671.20	J/mol×K	986.04	Joback Method
cpg	679.54	J/mol×K	1020.94	Joback Method
dvisc	0.0005528	Paxs	494.45	Joback Method
dvisc	0.0002685	Paxs	547.30	Joback Method

dvisc	0.0001481	Paxs	600.15	Joback Method
dvisc	0.0000899	Paxs	653.00	Joback Method
dvisc	0.0000589	Paxs	705.85	Joback Method
dvisc	0.0000409	Paxs	758.70	Joback Method
dvisc	0.0000297	Paxs	811.55	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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