Hexyl 4-hydroxybenzoate

Inchi: InChI=1S/C13H18O3/c1-2-3-4-5-10-16-13(15)11-6-8-12(14)9-7-11/h6-9,14H,2-5,10H2,1H
InchiKey: ULULAZKOCFNOIM-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CCCCCCOC(=O)c1ccc(O)cc1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	-217.55	kJ/mol	Joback Method
hf	-497.23	kJ/mol	Joback Method
hfus	32.04	kJ/mol	Joback Method
hvap	68.98	kJ/mol	Joback Method
log10ws	-3.95		Aqueous Solubility Prediction Method
logp	3.129		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	680.43	K	Joback Method
tc	892.73	K	Joback Method
tf	446.57	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.06	J/mol×K	680.43	Joback Method
cpg	513.11	J/mol×K	715.81	Joback Method
cpg	526.34	J/mol×K	751.20	Joback Method
cpg	538.80	J/mol×K	786.58	Joback Method
cpg	550.57	J/mol×K	821.96	Joback Method
cpg	561.70	J/mol×K	857.35	Joback Method
cpg	572.26	J/mol×K	892.73	Joback Method
dvisc	0.0005088	Pa×s	446.57	Joback Method
dvisc	0.0002287	Pa×s	485.55	Joback Method

dvisc	0.0001158	Pa×s	524.52	Joback Method
dvisc	0.0000644	Pa×s	563.50	Joback Method
dvisc	0.0000386	Pa×s	602.48	Joback Method
dvisc	0.0000247	Pa×s	641.45	Joback Method
dvisc	0.0000166	Pa×s	680.43	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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