Heptyl p-hydroxy benzoate

Other names:	Benzoic acid, 4-hydroxy-, heptyl ester
	Benzoic acid, p-hydroxy-, heptyl ester
	Heptyl 4-hydroxybenzoate
	Heptyl p-hydroxybenzoate
	Heptyl paraben
	NSC 309818
	Nipaheptyl
	Staypro WS 7
	n-Heptyl 4-hydroxybenzoate
	n-Heptyl p-hydroxybenzoate
	p-Hydroxybenzoic acid heptyl ester
	p-Oxybenzoesaureheptylester
Inchi:	InChI=1S/C14H20O3/c1-2-3-4-5-6-11-17-14(16)12-7-9-13(15)10-8-12/h7-10,15H,2-6,11H
InchiKey:	ZTJORNVITHUQJA-UHFFFAOYSA-N
Formula:	C14H20O3
SMILES:	CCCCCCCOC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	236.31

Physical Properties

Property code	Value	Unit	Source
af	0.8556		Cheméo Relay (1.0)
hf	-573.87	kJ/mol	Cheméo Relay (1.0)
hfus	34.63	kJ/mol	Joback Method
hvap	91.37	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-4.07		Aqueous Solubility Prediction Method
logp	3.519		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	601.88	K	Cheméo Relay (1.0)
tc	807.52	K	Cheméo Relay (1.0)
tf	346.61	K	Cheméo Relay (1.0)
vc	0.724	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.38	J/mol×K	703.31	Joback Method
cpg	565.93	J/mol×K	738.19	Joback Method
cpg	579.65	J/mol×K	773.07	Joback Method
cpg	592.60	J/mol×K	807.95	Joback Method
cpg	604.85	J/mol×K	842.84	Joback Method
cpg	616.46	J/mol×K	877.72	Joback Method
cpg	627.49	J/mol×K	912.60	Joback Method
dvisc	0.0004261	Pa×s	457.84	Joback Method
dvisc	0.0001888	Pa×s	498.75	Joback Method
dvisc	0.0000946	Pa×s	539.66	Joback Method
dvisc	0.0000523	Pa×s	580.57	Joback Method
dvisc	0.0000312	Pa×s	621.49	Joback Method
dvisc	0.0000199	Pa×s	662.40	Joback Method
dvisc	0.0000133	Pa×s	703.31	Joback Method

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1085127&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
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