

Benzoic acid, 4-hydroxy-, n-heptyl ester

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:	CCCCCCCCOC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	236.31
CAS:	1085-12-7

Physical Properties

Property code	Value	Unit	Source
gf	-209.13	kJ/mol	Joback Method
hf	-517.87	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	71.20	kJ/mol	Joback Method
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	703.31	K	Joback Method
tc	912.60	K	Joback Method
tf	457.84	K	Joback Method
vc	0.702	m3/kmol	Joback Method

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	580.58	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1085127&Units=SI
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/AqueousDataset002.xlsx
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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