2-Hydroxyethyl salicylate

Other names:	1,2-Ethylene glycol monosalicylate
	2-Hydroxybenzoic acid 2-hydroxyethyl ester
	2-Hydroxyethyl 2-hydroxybenzoate
	Benzoic acid, 2-hydroxy-, 2-hydroxyethyl ester
	Espirosal
	Ethylene glycol, monosalicylate
	Ethylene glycol, salicylate
	GL 7
	Glycol monosalicylate
	Glycol salicylate
	Glysal
	Monoglycol salicylate
	Norgesic
	Phlogont
	Rheumacyl
	Salicylic acid, 2-hydroxyethyl ester
	Sarocol
	Spirosal
	«beta»-Hydroxyethyl salicylate
	Â«betaÂ»-Hydroxyethyl salicylate
Inchi:	InChI=1S/C9H10O4/c10-5-6-13-9(12)7-3-1-2-4-8(7)11/h1-4,10-11H,5-6H2
InchiKey:	LVYLCBNXHHHPSB-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	O=C(OCCO)c1ccccc1O
Mol. weight [g/mol]:	182.17
CAS:	87-28-5

Physical Properties

Property code	Value	Unit	Source
gf	-388.05	kJ/mol	Joback Method
hf	-566.90	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	76.75	kJ/mol	Joback Method
log10ws	-1.16		Aqueous Solubility Prediction Method
logp	0.541		Crippen Method
mcvol	133.090	ml/mol	McGowan Method

pc	4665.71	kPa	Joback Method
rinpol	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
tb	681.09	K	Joback Method
tc	891.80	K	Joback Method
tf	462.31	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.48	J/mol×K	681.09	Joback Method
cpg	356.50	J/mol×K	716.21	Joback Method
cpg	364.98	J/mol×K	751.33	Joback Method
cpg	372.95	J/mol×K	786.45	Joback Method
cpg	380.48	J/mol×K	821.57	Joback Method
cpg	387.62	J/mol×K	856.68	Joback Method
cpg	394.41	J/mol×K	891.80	Joback Method
dvisc	0.0003499	Pa×s	462.31	Joback Method
dvisc	0.0001400	Pa×s	498.77	Joback Method
dvisc	0.0000635	Pa×s	535.24	Joback Method
dvisc	0.0000318	Pa×s	571.70	Joback Method
dvisc	0.0000173	Pa×s	608.16	Joback Method
dvisc	0.0000101	Pa×s	644.63	Joback Method
dvisc	0.0000063	Pa×s	681.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	439.20	K	1.70	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume