Phenylethyl salicylate

Other names:	«beta»-Phenylethyl salicylate
	Benzoic acid, 2-hydroxy-, 2-phenylethyl ester
	Benzylcarbinyl salicylate
	Phenethyl salicylate
	Phenylethyl salicyalte
	Salicylic acid, phenethyl ester
	2-Phenylethyl salicylate
Inchi:	InChI=1S/C15H14O3/c16-14-9-5-4-8-13(14)15(17)18-11-10-12-6-2-1-3-7-12/h1-9,16H,10
InchiKey:	YNMSDIQQNIRGDP-UHFFFAOYSA-N
Formula:	C15H14O3
SMILES:	O=C(OCCc1ccccc1)c1ccccc1O
Mol. weight [g/mol]:	242.27
CAS:	87-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-88.30	kJ/mol	Joback Method
hf	-301.98	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	75.71	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.792		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	752.87	K	Joback Method
tc	997.57	K	Joback Method
tf	495.53	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.53	J/mol×K	752.87	Joback Method
cpg	530.11	J/mol×K	793.65	Joback Method
cpg	542.69	J/mol×K	834.44	Joback Method
cpg	554.41	J/mol×K	875.22	Joback Method
cpg	565.37	J/mol×K	916.00	Joback Method
cpg	575.70	J/mol×K	956.78	Joback Method
cpg	585.51	J/mol×K	997.57	Joback Method
dvisc	0.0002445	Pa×s	495.53	Joback Method
dvisc	0.0001154	Pa×s	538.42	Joback Method
dvisc	0.0000609	Pa×s	581.31	Joback Method
dvisc	0.0000350	Pa×s	624.20	Joback Method
dvisc	0.0000217	Pa×s	667.09	Joback Method
dvisc	0.0000142	Pa×s	709.98	Joback Method
dvisc	0.0000098	Pa×s	752.87	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C87229&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume