

Phenylethyl salicylate

Other names:	«beta»-Phenylethyl salicylate Benzoic acid, 2-hydroxy-, 2-phenylethyl ester Benzylcarbiny 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(OCc1ccccc1)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	1934.00		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1966.00		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/molxK	752.87	Joback Method
cpg	530.11	J/molxK	793.65	Joback Method
cpg	542.69	J/molxK	834.44	Joback Method
cpg	554.41	J/molxK	875.22	Joback Method
cpg	565.37	J/molxK	916.00	Joback Method
cpg	575.70	J/molxK	956.78	Joback Method
cpg	585.51	J/molxK	997.57	Joback Method
dvisc	0.0002445	Paxs	495.53	Joback Method
dvisc	0.0001154	Paxs	538.42	Joback Method
dvisc	0.0000609	Paxs	581.31	Joback Method
dvisc	0.0000350	Paxs	624.20	Joback Method
dvisc	0.0000217	Paxs	667.09	Joback Method
dvisc	0.0000142	Paxs	709.98	Joback Method
dvisc	0.0000098	Paxs	752.87	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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