

Salicylic acid, methyl carbonate

Inchi:	InChI=1S/C9H8O5/c1-13-9(12)14-7-5-3-2-4-6(7)8(10)11/h2-5H,1H3,(H,10,11)
InchiKey:	IIHSMXMTENPGDE-UHFFFAOYSA-N
Formula:	C9H8O5
SMILES:	COC(=O)Oc1ccccc1C(=O)O
Mol. weight [g/mol]:	196.16
CAS:	14216-34-3

Physical Properties

Property code	Value	Unit	Source
gf	-476.98	kJ/mol	Joback Method
hf	-645.86	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	73.56	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.530		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	681.74	K	Joback Method
tc	888.91	K	Joback Method
tf	435.27	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.90	J/mol×K	681.74	Joback Method
cpg	344.87	J/mol×K	716.27	Joback Method
cpg	353.25	J/mol×K	750.80	Joback Method
cpg	361.04	J/mol×K	785.32	Joback Method
cpg	368.22	J/mol×K	819.85	Joback Method
cpg	374.80	J/mol×K	854.38	Joback Method
cpg	380.78	J/mol×K	888.91	Joback Method
dvisc	0.0010148	Pa×s	435.27	Joback Method
dvisc	0.0004977	Pa×s	476.35	Joback Method

dvisc	0.0002733	Pa×s	517.43	Joback Method
dvisc	0.0001639	Pa×s	558.50	Joback Method
dvisc	0.0001055	Pa×s	599.58	Joback Method
dvisc	0.0000718	Pa×s	640.66	Joback Method
dvisc	0.0000512	Pa×s	681.74	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14216343&Units=SI

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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