5-Methylsalicylic acid

Other names:	2-Hydroxy-5-methylbenzoic acid
	Benzoic acid, 2-hydroxy-5-methyl-
	«alpha»-Cresotinic acid
	p-Cresotic acid
	p-Cresotinic acid
	p-Homosalicylic acid
	2,5-Cresotic acid
	5-Methyl-2-hydroxybenzoic acid
	6-Hydroxy-m-toluic acid
	6-Hydroxy-3-methylbenzoic acid
	NSC 38518
Inchi:	InChI=1S/C8H8O3/c1-5-2-3-7(9)6(4-5)8(10)11/h2-4,9H,1H3,(H,10,11)
InchiKey:	DLGBEGBHXSAQOC-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	Cc1ccc(O)c(C(=O)O)c1
Mol. weight [g/mol]:	152.15
CAS:	89-56-5

Physical Properties

Property code	Value	Unit	Source
gf	-301.10	kJ/mol	Joback Method
hf	-425.51	kJ/mol	Joback Method
hfus	21.60	kJ/mol	Joback Method
hvap	72.78	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.399		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	5359.18	kPa	Joback Method
tb	640.77	K	Joback Method
tc	858.15	K	Joback Method
tf	422.00 ± 4.00	K	NIST Webbook
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.61	J/mol×K	640.77	Joback Method
cpg	284.67	J/mol×K	677.00	Joback Method
cpg	292.21	J/mol×K	713.23	Joback Method
cpg	299.28	J/mol×K	749.46	Joback Method
cpg	305.95	J/mol×K	785.69	Joback Method
cpg	312.29	J/mol×K	821.92	Joback Method
cpg	318.35	J/mol×K	858.15	Joback Method
dvisc	0.0005703	Pa×s	441.33	Joback Method
dvisc	0.0002373	Pa×s	474.57	Joback Method
dvisc	0.0001108	Pa×s	507.81	Joback Method
dvisc	0.0000568	Pa×s	541.05	Joback Method
dvisc	0.0000314	Pa×s	574.29	Joback Method
dvisc	0.0000186	Pa×s	607.53	Joback Method
dvisc	0.0000116	Pa×s	640.77	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C89565&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume