Benzoic acid, 5-(1,1-dimethylethyl)-2-hydroxy-

Other names: 5-(1,1-dimethylethyl)salicylic acid
Inchi: InChI=1S/C11H14O3/c1-11(2,3)7-4-5-9(12)8(6-7)10(13)14/h4-6,12H,1-3H3,(H,13,14)
InchiKey: XAICWTLLSRXZPB-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CC(C)(C)c1ccc(O)c(C(=O)O)c1
Mol. weight [g/mol]: 194.23
CAS: 16094-31-8

Physical Properties

Property code	Value	Unit	Source
gf	-273.00	kJ/mol	Joback Method
hf	-496.18	kJ/mol	Joback Method
hfus	21.95	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.388		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	706.18	K	Joback Method
tc	924.38	K	Joback Method
tf	477.56	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.54	J/mol×K	706.18	Joback Method
cpg	435.17	J/mol×K	742.55	Joback Method
cpg	445.14	J/mol×K	778.91	Joback Method
cpg	454.54	J/mol×K	815.28	Joback Method
cpg	463.45	J/mol×K	851.64	Joback Method
cpg	471.99	J/mol×K	888.01	Joback Method
cpg	480.23	J/mol×K	924.38	Joback Method
dvisc	0.0002717	Pa×s	477.56	Joback Method

dvisc	0.0001066	Pa×s	515.66	Joback Method
dvisc	0.0000476	Pa×s	553.77	Joback Method
dvisc	0.0000235	Pa×s	591.87	Joback Method
dvisc	0.0000127	Pa×s	629.97	Joback Method
dvisc	0.0000073	Pa×s	668.08	Joback Method
dvisc	0.0000045	Pa×s	706.18	Joback Method

Sources

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=C16094318&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume