

Salicylamide Me

Inchi:	InChI=1S/C9H11NO2/c1-10(2)9(12)7-5-3-4-6-8(7)11/h3-6,11H,1-2H3
InchiKey:	UBAYZMJYXBTDBB-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CN(C)C(=O)c1ccccc1O
Mol. weight [g/mol]:	165.19

Physical Properties

Property code	Value	Unit	Source
gf	-35.45	kJ/mol	Joback Method
hf	-214.92	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	59.71	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.094		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
tb	578.93	K	Joback Method
tc	806.07	K	Joback Method
tf	411.73	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.02	J/molxK	578.93	Joback Method
cpg	328.16	J/molxK	616.79	Joback Method
cpg	339.38	J/molxK	654.64	Joback Method
cpg	349.76	J/molxK	692.50	Joback Method
cpg	359.39	J/molxK	730.36	Joback Method
cpg	368.37	J/molxK	768.22	Joback Method
cpg	376.80	J/molxK	806.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R40493&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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