

Benzamide, 2-(acetyloxy)-

Other names:	Salicylamide, O-acetyl- O-Acetyl salicylamide Influina 2-(aminocarbonyl)phenyl acetate
Inchi:	InChI=1S/C9H9NO3/c1-6(11)13-8-5-3-2-4-7(8)9(10)12/h2-5H,1H3,(H2,10,12)
InchiKey:	KGHXFBVYXDFJGG-UHFFFAOYSA-N
Formula:	C9H9NO3
SMILES:	CC(=O)Oc1ccccc1C(N)=O
Mol. weight [g/mol]:	179.17
CAS:	5663-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-168.71	kJ/mol	Joback Method
hf	-327.62	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	65.11	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	0.711		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	639.67	K	Joback Method
tc	872.95	K	Joback Method
tf	435.48	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.08	J/mol×K	639.67	Joback Method
cpg	332.97	J/mol×K	678.55	Joback Method
cpg	343.08	J/mol×K	717.43	Joback Method
cpg	352.43	J/mol×K	756.31	Joback Method
cpg	361.04	J/mol×K	795.19	Joback Method

cpg	368.92	J/mol×K	834.07	Joback Method
cpg	376.08	J/mol×K	872.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5663718&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
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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