

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]:	179.18

Physical Properties

Property code	Value	Unit	Source
hf	-485.21	kJ/mol	Cheméo Relay (1.0)
hfus	22.30	kJ/mol	Joback Method
hvap	75.17	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
log10ws	-2.01		Cheméo Relay (1.0)
logp	0.711		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
tb	567.66	K	Cheméo Relay (1.0)
tf	363.87	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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