

Salacetamide

Other names:	Benzamide, N-acetyl-2-hydroxy- N-Acetylsalicylamide Arthrisin Ethrisin Labazyl Nacemide Rixamone Salicyl Salicylamide, N-acetyl- L-749 Acetsalicylamide Actylamide N-Acetyl-2-hydroxybenzamide 2-Hydroxy-N-acetylbenzamide NSC 40153
Inchi:	InChI=1S/C9H9NO3/c1-6(11)10-9(13)7-4-2-3-5-8(7)12/h2-5,12H,1H3,(H,10,11,13)
InchiKey:	JZWFDVDETGF GFC-UHFFFAOYSA-N
Formula:	C9H9NO3
SMILES:	CC(=O)NC(=O)c1ccccc1O
Mol. weight [g/mol]:	179.17
CAS:	487-48-9

Physical Properties

Property code	Value	Unit	Source
gf	-185.76	kJ/mol	Joback Method
hf	-341.56	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	0.668		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
tb	670.53	K	Joback Method
tc	906.37	K	Joback Method
tf	481.85	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.24	J/mol×K	670.53	Joback Method
cpg	346.16	J/mol×K	709.84	Joback Method
cpg	355.34	J/mol×K	749.14	Joback Method
cpg	363.87	J/mol×K	788.45	Joback Method
cpg	371.85	J/mol×K	827.75	Joback Method
cpg	379.35	J/mol×K	867.06	Joback Method
cpg	386.48	J/mol×K	906.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C487489&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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