Benzamide, N-acetyl-

Other names: N-Acetylbenzamide
Inchi: InChI=1S/C9H9NO2/c1-7(11)10-9(12)8-5-3-2-4-6-8/h2-6H,1H3,(H,10,11,12)
InchiKey: KGGRQKDGRGUWAT-UHFFFAOYSA-N
Formula: C9H9NO2
SMILES: CC(=O)NC(=O)c1ccccc1
Mol. weight [g/mol]: 163.17
CAS: 1575-95-7

Physical Properties

Property code	Value	Unit	Source
chs	-4454.59	kJ/mol	NIST Webbook
gf	-31.14	kJ/mol	Joback Method
hf	-164.25	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	0.963		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	589.91	K	Joback Method
tc	816.84	K	Joback Method
tf	370.13	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.82	J/mol×K	589.91	Joback Method
cpg	304.47	J/mol×K	627.73	Joback Method
cpg	315.28	J/mol×K	665.55	Joback Method
cpg	325.28	J/mol×K	703.37	Joback Method
cpg	334.51	J/mol×K	741.19	Joback Method
cpg	343.02	J/mol×K	779.02	Joback Method
cpg	350.83	J/mol×K	816.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1575957&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

Legend

chs:	Standard solid enthalpy of combustion
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