2-Amino-4-acetamino anisole

Other names: 4-Acetamino-2-aminoanisole
2-Amino-4-acetylaminoanisole
Acetamide, N-(3-amino-4-methoxyphenyl)-
2-Amino-4-acetamidoanisole
3'-amino-4'-methoxyacetanilide
Inchi: InChI=1S/C9H12N2O2/c1-6(12)11-7-3-4-9(13-2)8(10)5-7/h3-5H,10H2,1-2H3,(H,11,12)
InchiKey: SJWQCBCAGCEWCV-UHFFFAOYSA-N
Formula: C9H12N2O2
SMILES: COc1ccc(NC(C)=O)cc1N
Mol. weight [g/mol]: 180.20
CAS: 6375-47-9

Physical Properties

Property code	Value	Unit	Source
chs	-4702.50 ± 5.80	kJ/mol	NIST Webbook
gf	39.97	kJ/mol	Joback Method
hf	-173.04	kJ/mol	Joback Method
hfs	-554.00 ± 5.80	kJ/mol	NIST Webbook
hfus	25.41	kJ/mol	Joback Method
hvap	65.46	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.236		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	640.95	K	Joback Method
tc	866.84	K	Joback Method
tf	450.73	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.33	J/mol×K	640.95	Joback Method
cpg	367.26	J/mol×K	678.60	Joback Method

cpg	378.44	J/mol×K	716.25	Joback Method
cpg	388.87	J/mol×K	753.89	Joback Method
cpg	398.57	J/mol×K	791.54	Joback Method
cpg	407.55	J/mol×K	829.19	Joback Method
cpg	415.81	J/mol×K	866.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6375479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfs:	Solid phase 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