

Asulam

Other names:	4-Amino-benzolsulfonyl-methylcarbamat Asilan Asulfox F Asulox Asulox 40 Asulox F Carbamic acid, 4-aminobenzenesulfonyl-, methyl ester Carbamic acid, [(4-aminophenyl)sulfonyl]-, methyl ester Carbamic acid, sulfanilyl-, methyl ester Jonnix M and B 9057 MB 9057 Methyl (4-aminophenylsulfonyl)carbamate Methyl 4-aminobenzenesulfonylcarbamate Methyl 4-aminobenzenesulphonyl carbamate Methyl 4-aminophenylsulphonyl carbamate Methyl N-(4-aminobenzenesulfonyl)carbamate Methyl p-aminobenzenesulfonylcarbamate Methyl sulfanilyl carbamate N1-Methoxycarbonylsulfanilamide
Inchi:	InChI=1S/C8H10N2O4S/c1-14-8(11)10-15(12,13)7-4-2-6(9)3-5-7/h2-5H,9H2,1H3,(H,10,1
InchiKey:	VGPYEHKOIGNJKV-UHFFFAOYSA-N
Formula:	C8H10N2O4S
SMILES:	COC(=O)NS(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	230.24
CAS:	3337-71-1

Physical Properties

Property code	Value	Unit	Source
gf	-427.36	kJ/mol	Joback Method
hf	-594.28	kJ/mol	Joback Method
hfus	34.59	kJ/mol	Joback Method
hvap	81.21	kJ/mol	Joback Method
log10ws	-1.66		Aqueous Solubility Prediction Method
logp	0.314		Crippen Method
mcvol	155.310	ml/mol	McGowan Method

pc	5109.34	kPa	Joback Method
tb	660.87	K	Joback Method
tc	880.81	K	Joback Method
tf	417.30 ± 0.20	K	NIST Webbook
vc	0.590	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.95	J/mol×K	660.87	Joback Method
cpg	400.21	J/mol×K	697.53	Joback Method
cpg	410.62	J/mol×K	734.18	Joback Method
cpg	420.17	J/mol×K	770.84	Joback Method
cpg	428.86	J/mol×K	807.50	Joback Method
cpg	436.68	J/mol×K	844.16	Joback Method
cpg	443.63	J/mol×K	880.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3337711&Units=SI

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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