SULPHAUREA

Other names: (4-aminophenyl)sulfonylurea
1-(4-Aminobenzenesulfonyl)urea
1-Sulfanilylurea
1-Sulfanylurea
4-Amino-N-(aminocarbonyl)benzenesulfonamide
4-Sulfacarbamide
A 435
Benzenesulfonamide, 4-amino-N-(aminocarbonyl)-
Euvernil
N-Sulfanilcarbamide
NSC 78438
Sulfanilamide, N1-carbamoyl-
Sulfanilcarbamid
Sulfanilylurea
Sulfanylharnstoff
Sulfanyluree
Sulfaurea
Uractyl
Uramid
Urea, sulfanilyl-
Urenil
Urosulfan
Urosulfane
p-Aminobenzenesulfonylurea

Inchi: InChI=1S/C7H9N3O3S/c8-5-1-3-6(4-2-5)14(12,13)10-7(9)11/h1-4H,8H2,(H3,9,10,11)

InchiKey: WVAKABMNNSMCDK-UHFFFAOYSA-N

Formula: C7H9N3O3S

SMILES: NC(=O)NS(=O)(=O)c1ccc(N)cc1

Mol. weight [g/mol]: 215.23

Physical Properties

Property code	Value	Unit	Source
hfus	36.01	kJ/mol	Joback Method
hvap	104.62	kJ/mol	Cheméo Relay (1.0)
ie	8.28	eV	Cheméo Relay (1.0)
log10ws	-1.97		Aqueous Solubility Prediction Method

logp	-0.374		Crippen Method
mcvol	145.330	ml/mol	McGowan Method
tf	447.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.20	J/mol×K	688.10	Joback Method
cpg	380.26	J/mol×K	726.97	Joback Method
cpg	389.41	J/mol×K	765.85	Joback Method
cpg	397.67	J/mol×K	804.72	Joback Method
cpg	405.03	J/mol×K	843.59	Joback Method
cpg	411.53	J/mol×K	882.47	Joback Method
cpg	417.17	J/mol×K	921.34	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C547444&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg: Ideal gas heat capacity
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
tf: Normal melting (fusion) point