Sulfacarbamide

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
	Sulphaurea
	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
CAS:	547-44-4

Physical Properties

Property code	Value	Unit	Source
gf	-264.33	kJ/mol	Joback Method
hf	-407.63	kJ/mol	Joback Method

hfus	36.01	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-1.97		Aqueous Solubility Prediction Method
logp	-0.374		Crippen Method
mcvol	145.330	ml/mol	McGowan Method
pc	6620.58	kPa	Joback Method
rinpol	2040.40		NIST Webbook
rinpol	2040.40		NIST Webbook
tb	688.10	K	Joback Method
tc	921.34	K	Joback Method
tf	515.26	K	Joback Method
vc	0.544	m3/kmol	Joback Method

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

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/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C547444&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume