(4-aminophenyl)sulfonylthiourea

Inchi: InChI=1S/C7H9N3O2S2/c8-5-1-3-6(4-2-5)14(11,12)10-7(9)13/h1-4H,8H2,(H3,9,10,13)
InchiKey: UEMLYRZWLVXWRU-UHFFFAOYSA-N
Formula: C7H9N3O2S2
SMILES: NC(=S)NS(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 231.30

Physical Properties

Property code	Value	Unit	Source
gf	-18.35	kJ/mol	Joback Method
hf	-148.55	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-2.24		Aqueous Solubility Prediction Method
logp	-0.209		Crippen Method
mcvol	155.810	ml/mol	McGowan Method
pc	6944.44	kPa	Joback Method
tb	704.27	K	Joback Method
tc	952.98	K	Joback Method
tf	453.65	K	Aqueous Solubility Prediction Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.13	J/mol×K	704.27	Joback Method
cpg	390.76	J/mol×K	745.72	Joback Method
cpg	399.45	J/mol×K	787.17	Joback Method
cpg	407.28	J/mol×K	828.62	Joback Method
cpg	414.31	J/mol×K	870.07	Joback Method
cpg	420.61	J/mol×K	911.53	Joback Method
cpg	426.22	J/mol×K	952.98	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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