phenbutamide

Inchi: InChI=1S/C11H16N2O3S/c1-2-3-9-12-11(14)13-17(15,16)10-7-5-4-6-8-10/h4-8H,2-3,9H2
InchiKey: AFOGBLYPWJJVAL-UHFFFAOYSA-N
Formula: C11H16N2O3S
SMILES: CCCCNC(=O)NS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 256.33

Physical Properties

Property code	Value	Unit	Source
gf	-264.53	kJ/mol	Joback Method
hf	-492.83	kJ/mol	Joback Method
hfus	41.46	kJ/mol	Joback Method
hvap	80.61	kJ/mol	Joback Method
log10ws	-3.05		Aqueous Solubility Prediction Method
logp	1.475		Crippen Method
mcvol	191.710	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	679.75	K	Joback Method
tc	884.07	K	Joback Method
tf	433.96	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.49	J/mol×K	679.75	Joback Method
cpg	521.20	J/mol×K	713.80	Joback Method
cpg	533.95	J/mol×K	747.86	Joback Method
cpg	545.74	J/mol×K	781.91	Joback Method
cpg	556.61	J/mol×K	815.96	Joback Method
cpg	566.58	J/mol×K	850.01	Joback Method
cpg	575.67	J/mol×K	884.07	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

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