carbutamide

Inchi: InChI=1S/C11H17N3O3S/c1-2-3-8-13-11(15)14-18(16,17)10-6-4-9(12)5-7-10/h4-7H,2-3,
InchiKey: VDTNNGKXZGSZIP-UHFFFAOYSA-N
Formula: C11H17N3O3S
SMILES: CCCCNC(=O)NS(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 271.34

Physical Properties

Property code	Value	Unit	Source
gf	-207.71	kJ/mol	Joback Method
hf	-470.51	kJ/mol	Joback Method
hfus	46.27	kJ/mol	Joback Method
hvap	91.91	kJ/mol	Joback Method
log10ws	-2.18		Aqueous Solubility Prediction Method
logp	1.057		Crippen Method
mcvol	201.690	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	757.26	K	Joback Method
tc	969.26	K	Joback Method
tf	417.40	K	Aqueous Solubility Prediction Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.42	J/mol×K	757.26	Joback Method
cpg	579.87	J/mol×K	792.59	Joback Method
cpg	591.31	J/mol×K	827.93	Joback Method
cpg	601.76	J/mol×K	863.26	Joback Method
cpg	611.24	J/mol×K	898.60	Joback Method
cpg	619.77	J/mol×K	933.93	Joback Method
cpg	627.38	J/mol×K	969.26	Joback Method

Sources

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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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