benzylurea

Inchi: InChI=1S/C8H10N2O/c9-8(11)10-6-7-4-2-1-3-5-7/h1-5H,6H2,(H3,9,10,11)
InchiKey: RJNJWHFSKNJCTB-UHFFFAOYSA-N
Formula: C8H10N2O
SMILES: NC(=O)NCc1ccccc1
Mol. weight [g/mol]: 150.18

Physical Properties

Property code	Value	Unit	Source
gf	155.81	kJ/mol	Joback Method
hf	2.76	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	59.50	kJ/mol	Joback Method
log10ws	-0.95		Estimated Solubility Method
log10ws	-0.95		Aqueous Solubility Prediction Method
logp	0.855		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	585.69	K	Joback Method
tc	817.28	K	Joback Method
tf	421.65	K	Aqueous Solubility Prediction Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.51	J/mol×K	585.69	Joback Method
cpg	299.27	J/mol×K	624.29	Joback Method
cpg	310.17	J/mol×K	662.89	Joback Method
cpg	320.27	J/mol×K	701.48	Joback Method
cpg	329.58	J/mol×K	740.08	Joback Method
cpg	338.17	J/mol×K	778.68	Joback Method
cpg	346.07	J/mol×K	817.28	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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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