Urea, (4-ethoxyphenyl)-

Other names:	1-(4-Ethoxyphenyl)urea
	4-Ethoxyphenylurea
	Dulcin
	Dulcine
	Dulein
	N-(4-Ethoxyphenyl)urea
	NCI-C02073
	NSC 1839
	Phenethylcarbamid
	Phenetolcarbamide
	Sucrol
	Suesstoff
	Urea, (p-ethoxyphenyl)-
	Valzin
	p-Aethoxyphenylharnstoff
	p-Ethoxyfenylmocovina
	p-Ethoxyphenylurea
	p-Phenethylurea
	p-Phenetolcarbamid
	p-Phenetolcarbamide
	p-Phenetolecarbamide
	p-Phenetylurea
Inchi:	InChI=1S/C9H12N2O2/c1-2-13-8-5-3-7(4-6-8)11-9(10)12/h3-6H,2H2,1H3,(H3,10,11,12)
InchiKey:	GGLIEWRLXDLBBF-UHFFFAOYSA-N
Formula:	C9H12N2O2
SMILES:	CCOc1ccc(NC(N)=O)cc1
Mol. weight [g/mol]:	180.20
CAS:	150-69-6

Physical Properties

Property code	Value	Unit	Source
gf	49.60	kJ/mol	Joback Method
hf	-161.57	kJ/mol	Joback Method
hfus	25.80	kJ/mol	Joback Method
hvap	64.80	kJ/mol	Joback Method
log10ws	-2.17		Estimated Solubility Method

log10ws	-2.17		Aqueous Solubility Prediction Method
logp	1.576		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	635.97	K	Joback Method
tc	860.95	K	Joback Method
tf	446.65	K	Aqueous Solubility Prediction Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.51	J/mol×K	635.97	Joback Method
cpg	368.64	J/mol×K	673.47	Joback Method
cpg	379.97	J/mol×K	710.96	Joback Method
cpg	390.52	J/mol×K	748.46	Joback Method
cpg	400.31	J/mol×K	785.96	Joback Method
cpg	409.35	J/mol×K	823.45	Joback Method
cpg	417.67	J/mol×K	860.95	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C150696&Units=SI
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

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