(P-ETHOXYPHENYL)UREA

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]: 180.21

Physical Properties

Property code	Value	Unit	Source
af	0.7368		Cheméo Relay (1.0)
hf	-344.03	kJ/mol	Cheméo Relay (1.0)
hfus	25.80	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Cheméo Relay (1.0)
ie	7.89	eV	Cheméo Relay (1.0)
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	576.40	K	Cheméo Relay (1.0)
tc	820.52	K	Cheméo Relay (1.0)
tf	446.65	K	Aqueous Solubility Prediction 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C150696&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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