

Fenuron

Other names:	1,1-Dimethyl-3-phenylurea
	1-Phenyl-3,3-dimethylurea
	3-Phenyl-1,1-dimethylurea
	Amicure UR
	Dibar
	Dybar
	Dyhard RU 300
	Dyhard UR 300
	Falisilvan
	Fenidin
	Fenulon
	Fikure 62U
	N,N-Dimethyl-N'-phenylurea
	N-Phenyl-N',N'-dimethylurea
	Omicure 94
	PDU
	PUD
	PUD (Herbicide)
	Urea, 1,1-dimethyl-3-phenyl-
	Urea, N,N-dimethyl-N'-phenyl-
Inchi:	InChI=1S/C9H12N2O/c1-11(2)9(12)10-8-6-4-3-5-7-8/h3-7H,1-2H3,(H,10,12)
InchiKey:	XXOYNJXVWVNOOJ-UHFFFAOYSA-N
Formula:	C9H12N2O
SMILES:	CN(C)C(=O)Nc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	101-42-8

Physical Properties

Property code	Value	Unit	Source
chs	-5054.30 ± 4.20	kJ/mol	NIST Webbook
gf	208.56	kJ/mol	Joback Method
hf	15.86	kJ/mol	Joback Method
hfs	-203.00 ± 4.20	kJ/mol	NIST Webbook
hfus	22.83	kJ/mol	Joback Method
hvap	53.13	kJ/mol	Joback Method
log10ws	-1.60		Estimated Solubility Method

log10ws	-1.60		Aqueous Solubility Prediction Method
logp	1.780		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	548.48	K	Joback Method
tc	764.08	K	Joback Method
tf	406.38 ± 0.20	K	NIST Webbook
tf	406.00 ± 0.20	K	NIST Webbook
tf	406.53	K	Aqueous Solubility Prediction Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.50	J/mol×K	548.48	Joback Method
cpg	326.22	J/mol×K	584.41	Joback Method
cpg	339.01	J/mol×K	620.35	Joback Method
cpg	350.93	J/mol×K	656.28	Joback Method
cpg	362.01	J/mol×K	692.21	Joback Method
cpg	372.29	J/mol×K	728.14	Joback Method
cpg	381.83	J/mol×K	764.08	Joback Method
hfust	22.81	kJ/mol	404.80	NIST Webbook
hfust	22.81	kJ/mol	404.80	NIST Webbook
sfust	59.77	J/mol×K	404.80	NIST Webbook

Sources

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

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C101428&Units=SI>

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

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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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