Isoproturon

Other names:	1,1-dimethyl-3-(4-propan-2-ylphenyl)urea
	3-(4-Isopropylphenyl)-1,1-dimethylurea
	Alon
	Arelon
	Arelon R
	Belgran
	CGA-18731
	CL 12150
	DPX 6774
	Graminon
	HOE 16410
	Hytane 500L
	IP 50
	IP-Flo
	IPU Stefes
	N'-(4-Isopropylphenyl)-N,N-dimethylurea
	N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea
	N-(4-Isopropylphenyl)-N',N'-dimethylharnstoff
	N-(4-Isopropylphenyl)-N',N'-dimethylurea
	N-4-Isopropylphenyl-N,N-dimethylurea
	Nocilon
	Protugan
	Tolkan
	Tolken
	Urea, 1,1-dimethyl-3-(p-isopropylphenyl)-
	Urea, 3-p-cumenyl-1,1-dimethyl-
	Urea, N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]-
Inchi:	InChI=1S/C12H18N2O/c1-9(2)10-5-7-11(8-6-10)13-12(15)14(3)4/h5-9H,1-4H3,(H,13,15)
InchiKey:	PUIYMUZLKQOUOZ-UHFFFAOYSA-N
Formula:	C12H18N2O
SMILES:	CC(C)c1ccc(NC(=O)N(C)C)cc1
Mol. weight [g/mol]:	206.28
CAS:	34123-59-6

Physical Properties

Property code	Value	Unit	Source

gf	221.75	kJ/mol	Joback Method
hf	-62.81	kJ/mol	Joback Method
hfus	26.68	kJ/mol	Joback Method
hvap	60.08	kJ/mol	Joback Method
log10ws	-3.54		Estimated Solubility Method
log10ws	-3.52		Aqueous Solubility Prediction Method
logp	2.904		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
tb	621.66	K	Joback Method
tc	832.03	K	Joback Method
tf	430.81 ± 0.20	K	NIST Webbook
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.31	J/mol×K	621.66	Joback Method
cpg	473.02	J/mol×K	656.72	Joback Method
cpg	487.74	J/mol×K	691.78	Joback Method
cpg	501.51	J/mol×K	726.84	Joback Method
cpg	514.38	J/mol×K	761.90	Joback Method
cpg	526.39	J/mol×K	796.97	Joback Method
cpg	537.59	J/mol×K	832.03	Joback Method
hfust	21.33	kJ/mol	427.40	NIST Webbook
hfust	33.87	kJ/mol	430.40	NIST Webbook

Sources

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=C34123596&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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume