Acetohexamide

Other names:	1-(p-Acetylbenzenesulfonyl)-3-Cyclohexylurea
	1-[(p-Acetylphenyl)sulfonyl]-3-cyclohexylurea
	4-Acetyl-N-[(cyclohexylamino)-carbonyl]benzenesulfonamide
	Acetohexamid
	Benzenesulfonamide, 4-acetyl-N-[(cyclohexylamino)carbonyl]-
	Dimelin
	Dimelor
	Dymelor
	Gamadiabet
	Hypoglicil
	Metaglucina
	Minoral
	N-(p-Acetylbenzenesulfonyl)-N'-cyclohexylurea
	N-(p-Acetylphenylsulfonyl)-N'-cyclohexylurea
	NCI-C03247
	Ordimel
	Tsiklamid
	U-14812
	Urea, 1-[(p-acetylphenyl)sulfonyl]-3-cyclohexyl-
Inchi:	InChI=1S/C15H20N2O4S/c1-11(18)12-7-9-14(10-8-12)22(20,21)17-15(19)16-13-5-3-2-4-
InchiKey:	VGZSUPCWNCWDAN-UHFFFAOYSA-N
Formula:	C15H20N2O4S
SMILES:	CC(=O)c1ccc(S(=O)(=O)NC(=O)NC2CCCCC2)cc1
Mol. weight [g/mol]:	324.39
CAS:	968-81-0

Physical Properties

Property code	Value	Unit	Source
gf	-344.95	kJ/mol	Joback Method
hf	-645.12	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	97.35	kJ/mol	Joback Method
log10ws	-2.06		Aqueous Solubility Prediction Method
logp	2.210		Crippen Method
mcvol	238.780	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method

tb	849.67	K	Joback Method
tc	1078.06	K	Joback Method
tf	461.65	K	Aqueous Solubility Prediction Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.77	J/mol×K	849.67	Joback Method
cpg	745.60	J/mol×K	887.74	Joback Method
cpg	757.92	J/mol×K	925.80	Joback Method
cpg	768.77	J/mol×K	963.87	Joback Method
cpg	778.19	J/mol×K	1001.93	Joback Method
cpg	786.23	J/mol×K	1040.00	Joback Method
cpg	792.92	J/mol×K	1078.06	Joback Method
hfust	41.08	kJ/mol	457.00	NIST Webbook

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C968810&Units=SI

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