Nimesulide

Other names:	4'-Nitro-2'-phenoxymethanesulfonanilide
	4-Nitro-2-phenoxy-methanesulfonanilide
	Aulin
	Flogovital
	Mesulid
	Methanesulfonamide, N-(4-nitro-2-phenoxyphenyl)-
	Methanesulfonanilide, 4'-nitro-2'-phenoxy-
	N-(4-Nitro-2-phenoxyphenyl)methanesulfonamide
	N-(4-nitro-2-phenoxyphenyl)methanesulfonamide (nimesulide)
	N-[4-nitro-2-(phenoxy)phenyl]methanesulfonamide
	Nimed
	Nisulid
	R-805
	Sulidene
Inchi:	InChI=1S/C13H12N2O5S/c1-21(18,19)14-12-8-7-10(15(16)17)9-13(12)20-11-5-3-2-4-6-1
InchiKey:	HYWYRSMBCFDLJT-UHFFFAOYSA-N
Formula:	C13H12N2O5S
SMILES:	CS(=O)(=O)Nc1ccc([N+](=O)[O-])cc1Oc1ccccc1
Mol. weight [g/mol]:	308.31
CAS:	51803-78-2

Physical Properties

Property code	Value	Unit	Source
gf	-184.46	kJ/mol	Joback Method
hf	-404.39	kJ/mol	Joback Method
hfus	45.76	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-4.49		Aqueous Solubility Prediction Method
logp	2.759		Crippen Method
mcvol	207.870	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	832.37	K	Joback Method
tc	1080.24	K	Joback Method
tf	416.90	K	Aqueous Solubility Prediction Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.53	J/mol×K	832.37	Joback Method
cpg	591.83	J/mol×K	873.68	Joback Method
cpg	601.72	J/mol×K	914.99	Joback Method
cpg	610.22	J/mol×K	956.31	Joback Method
cpg	617.36	J/mol×K	997.62	Joback Method
cpg	623.16	J/mol×K	1038.93	Joback Method
cpg	627.66	J/mol×K	1080.24	Joback Method
hfust	37.30	kJ/mol	422.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51803782&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

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

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