Oryzalin

Other names:	3,5-Dinitro-N4,N4-dipropylsulfanilamide
	4-(Dipropylamino)-3,5-dinitrobenzenesulfonamide
	4-(N,N-dipropylamino)-3,5-dinitrobenzenesulphonamide
	Benzenesulfonamide, 4-(dipropylamino)-3,5-dinitro-
	Dirimal
	EL 119
	N4,N4-Dipropyl-3,5-dinitrosulfanilamide
	NSC 648479
	Rizelan
	Rycelan
	Rycelon
	Ryzelan
	Sulfanilamide, 3,5-dinitro-N4,N4-dipropyl-
	Surflan
Inchi:	InChI=1S/C12H18N4O6S/c1-3-5-14(6-4-2)12-10(15(17)18)7-9(23(13,21)22)8-11(12)16(1
InchiKey:	UNAHYJYOSSSJHH-UHFFFAOYSA-N
Formula:	C12H18N4O6S
SMILES:	CCCN(CCC)c1c([N+](=O)[O-])cc(S(N)(=O)=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	346.36
CAS:	19044-88-3

Physical Properties

Property code	Value	Unit	Source
gf	-86.53	kJ/mol	Joback Method
hf	-462.44	kJ/mol	Joback Method
hfus	62.03	kJ/mol	Joback Method
hvap	111.07	kJ/mol	Joback Method
log10ws	-5.16		Aqueous Solubility Prediction Method
log10ws	-5.16		Estimated Solubility Method
logp	1.777		Crippen Method
mcvol	239.070	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	2619.00		NIST Webbook
tb	952.01	K	Joback Method
tc	1192.53	K	Joback Method

tf	415.48 ± 0.20	K	NIST Webbook
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.32	J/mol×K	952.01	Joback Method
cpg	744.75	J/mol×K	992.10	Joback Method
cpg	752.94	J/mol×K	1032.18	Joback Method
cpg	759.93	J/mol×K	1072.27	Joback Method
cpg	765.76	J/mol×K	1112.36	Joback Method
cpg	770.46	J/mol×K	1152.44	Joback Method
cpg	774.09	J/mol×K	1192.53	Joback Method
hfust	38.48	kJ/mol	414.80	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19044883&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume