Nitralin

Other names:	Benzenamine, 4-(methylsulfonyl)-2,6-dinitro-N,N-dipropyl-
	Aniline, 4-(methylsulfonyl)-2,6-dinitro-N,N-dipropyl-
	N,N-Dipropyl-4-methylsulfonyl-2,6-dinitroaniline
	Nitraline
	Planavin
	Planavin 75
	Planuin
	Niralin
	SD 11831
	4-(Methylsulfonyl)-2,6-dinitro-N,N-dipropylbenzeneamine
	4-(Methylsulfonyl)-2,6-dinitro-N,N-dipropylbenzenamine
	2,6-Dinitro-4-methylsulfonyl-N,N-dipropylaniline
	4-Methylsulphonyl-2,6-dinitro-N,N-dipropylaniline
Inchi:	InChI=1S/C13H19N3O6S/c1-4-6-14(7-5-2)13-11(15(17)18)8-10(23(3,21)22)9-12(13)16(1
InchiKey:	UMKANAFDOQQUKE-UHFFFAOYSA-N
Formula:	C12H16N3O6S
SMILES:	CCCN(CCC)c1c([N+](=O)[O-])cc(S(C)(=O)=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	330.34
CAS:	4726-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-144.56	kJ/mol	Joback Method
hf	-516.87	kJ/mol	Joback Method
hfus	59.42	kJ/mol	Joback Method
hvap	102.65	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	2.533		Crippen Method
mcvol	243.180	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	2447.00		NIST Webbook
tb	902.36	K	Joback Method
tc	1134.43	K	Joback Method
tf	424.83 ± 0.20	K	NIST Webbook
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.03	J/mol×K	902.36	Joback Method
cpg	747.29	J/mol×K	941.04	Joback Method
cpg	757.31	J/mol×K	979.72	Joback Method
cpg	766.13	J/mol×K	1018.39	Joback Method
cpg	773.80	J/mol×K	1057.07	Joback Method
cpg	780.35	J/mol×K	1095.75	Joback Method
cpg	785.82	J/mol×K	1134.43	Joback Method
hfust	28.05	kJ/mol	424.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4726141&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume