Ethalfluralin

Other names:	Benzenamine, N-ethyl-N-(2-methyl-2-propen-1-yl)-2,6-dinitro-4-(trifluoromethyl)- Benzenamine, N-ethyl-N-(2-methyl-2-propenyl)-2,6-dinitro-4-(trifluoromethyl)- Buvilan EL 161 Edge Ethafluralin N-Ethyl-N-(2-methyl-2-propenyl)-2,6-dinitro-4-(trifluoromethyl)benzenamine Sonalan p-Toluidine, 2,6-dinitro-N-ethyl-N-(2-methyl-2-propenyl)-«alpha»,«alpha»,«alpha»-trifluoro-
Inchi:	p-Toluidine, 2,6-dinitro-N-ethyl-N-(2-methyl-2-propenyl)-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro- InChI=1S/C13H14F3N3O4/c1-4-17(7-8(2)3)12-10(18(20)21)5-9(13(14,15)16)6-11(12)19(
InchiKey:	PTFJIKYUEPWBMS-UHFFFAOYSA-N
Formula:	C13H14F3N3O4
SMILES:	C=C(C)CN(CC)c1c([N+](=O)[O-])cc(C(F)(F)F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	333.26
CAS:	55283-68-6

Physical Properties

Property code	Value	Unit	Source
gf	-178.32	kJ/mol	Joback Method
hf	-544.96	kJ/mol	Joback Method
hfus	47.28	kJ/mol	Joback Method
hvap	79.68	kJ/mol	Joback Method
log10ws	-6.12		Aqueous Solubility Prediction Method
log10ws	-6.12		Estimated Solubility Method
logp	3.924		Crippen Method
mcvol	216.100	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1648.00		NIST Webbook
tb	845.72	K	Joback Method
tc	1076.02	K	Joback Method
tf	328.65	K	Aqueous Solubility Prediction Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.52	J/mol×K	845.72	Joback Method
cpg	657.71	J/mol×K	884.10	Joback Method
cpg	668.06	J/mol×K	922.49	Joback Method
cpg	677.65	J/mol×K	960.87	Joback Method
cpg	686.58	J/mol×K	999.25	Joback Method
cpg	694.95	J/mol×K	1037.64	Joback Method
cpg	702.84	J/mol×K	1076.02	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
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=C55283686&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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