

Benfluralin

Other names:	Balan
	Balfin
	Banafine
	Benalan
	Benefex
	Benefin
	Benephin
	Benfluraline
	Benzenamine, N-butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)-
	Bethrodine
	Binnell
	Blulan
	Bonalan
	Carpidor
	EL-110
	Emblem
	Flubalex
	L 54521
	N-Butyl-2,6-dinitro-N-ethyl-4-trifluoromethylaniline
	N-Butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)benzenamine
	N-Butyl-N-ethyl-2,6-dinitro-4-trifluoromethylaniline
	N-Butyl-N-ethyl-«alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-p-toluidine
	N-Butyl-N-ethyl-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-2,6-dinitro-p-toluidine
	Quilan
	p-Toluidine, N-butyl-N-ethyl-«alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-
	p-Toluidine, N-butyl-N-ethyl-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-2,6-dinitro-
	«alpha»,«alpha»,«alpha»-Trifluoro-2,6-dinitro-N,N-ethylbutyl-p-toluidine
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trifluoro-2,6-dinitro-N,N-ethylbutyl-p-toluidine
Inchi:	InChI=1S/C13H16F3N3O4/c1-3-5-6-17(4-2)12-10(18(20)21)7-9(13(14,15)16)8-11(12)19
InchiKey:	SMDHCQAYESWHAE-UHFFFAOYSA-N
Formula:	C13H16F3N3O4
SMILES:	CCCCN(CC)c1c([N+](=O)[O-])cc(C(F)(F)F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	335.28
CAS:	1861-40-1

Physical Properties

Property code	Value	Unit	Source
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gf	-257.61	kJ/mol	Joback Method
hf	-660.60	kJ/mol	Joback Method
hfus	49.87	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-5.53		Aqueous Solubility Prediction Method
log10ws	-5.53		Estimated Solubility Method
logp	4.148		Crippen Method
mcvol	220.400	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	849.16	K	Joback Method
tc	1073.60	K	Joback Method
tf	338.72 ± 0.20	K	NIST Webbook
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.85	J/mol×K	1036.19	Joback Method
cpg	673.72	J/mol×K	849.16	Joback Method
cpg	685.33	J/mol×K	886.57	Joback Method
cpg	696.07	J/mol×K	923.97	Joback Method
cpg	706.01	J/mol×K	961.38	Joback Method
cpg	715.24	J/mol×K	998.78	Joback Method
cpg	731.90	J/mol×K	1073.60	Joback Method
hfust	36.50	kJ/mol	338.50	NIST Webbook

Sources

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=C1861401&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

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

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