Benzenamine, N-butyl-N-ethyl-2,6-dinitro-4-(trifluoromethyl)-

Other names: Balan
Balfin
Banafine
Benalan
Benefex
Benefin
Benephin
Benfluraline
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
Quilan
benfluralin
p-Toluidine, N-butyl-N-ethyl-«alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-
«alpha»,«alpha»,«alpha»-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

Physical Properties

Property code	Value	Unit	Source
hfus	49.87	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
rinpol	1670.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	577.87	K	Cheméo Relay (1.0)
tf	338.72 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	723.85	J/mol×K	1036.19	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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1861401&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point