Fluchloralin

Other names: Benzenamine, N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)-
p-Toluidine, N-(2-chloroethyl)-«alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-N-propyl-
Basalin
BAS 392 04 H
BAS 3921
BAS 3921 H
BAS 3924H
p-Toluidine, N-(2-chloroethyl)-2,6-dinitro-N-propyl-«alpha»,«alpha»,«alpha»-trifluoro-
BAS 3920
BAS 3922
N-(2-Chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)aniline
N-(2-Chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzenamine
N-(2-Chloroethyl)-«alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-N-propyl-p-toluidine
N-Propyl-N-(2-chloroethyl)-2,6-dinitro-4-trifluoromethylaniline
N-Propyl-N-(2-chloroethyl)-«alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-p-toluidine
N-(2-chloroethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzeneamine

Inchi: InChI=1S/C12H13ClF3N3O4/c1-2-4-17(5-3-13)11-9(18(20)21)6-8(12(14,15)16)7-10(11)1

InchiKey: MNFMIVVPXOGUMX-UHFFFAOYSA-N

Formula: C12H13ClF3N3O4

SMILES: CCCN(CCCl)c1c([N+](=O)[O-])cc(C(F)(F)F)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 355.70

CAS: 33245-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-277.96	kJ/mol	Joback Method
hf	-655.70	kJ/mol	Joback Method
hfus	51.48	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.977		Crippen Method
mcvol	218.550	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
tb	863.71	K	Joback Method
tc	1093.61	K	Joback Method
tf	320.88 ± 0.20	K	NIST Webbook
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.18	J/mol×K	1055.29	Joback Method
cpg	639.45	J/mol×K	863.71	Joback Method
cpg	649.63	J/mol×K	902.03	Joback Method
cpg	659.01	J/mol×K	940.34	Joback Method
cpg	667.67	J/mol×K	978.66	Joback Method
cpg	675.70	J/mol×K	1016.98	Joback Method
cpg	690.21	J/mol×K	1093.61	Joback Method
hfust	23.08	kJ/mol	318.40	NIST Webbook

Sources

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=C33245395&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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume