Profluralin

Other names:	Benzenamine, N-(cyclopropylmethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)- p-Toluidine, N-(cyclopropylmethyl)-«alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-N-propyl- CG-10832 CGA 10832 ER 5461 SGA 10832 Tolban Profluraline N-(Cyclopropylmethyl)-2,6-dinitro-n-propyl-4-(trifluoromethyl)aniline B 4576 N-Cyclopropylmethyl-N-n-propyl-4-trifluoromethyl-2,6-dinitroaniline Pregard N-(cyclopropylmethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzenamine
Inchi:	InChI=1S/C14H16F3N3O4/c1-2-5-18(8-9-3-4-9)13-11(19(21)22)6-10(14(15,16)17)7-12(1
InchiKey:	ITVQAKZNYJEWKS-UHFFFAOYSA-N
Formula:	C14H16F3N3O4
SMILES:	CCCN(CC1CC1)c1c([N+](=O)[O-])cc(C(F)(F)F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	347.29
CAS:	26399-36-0

Physical Properties

Property code	Value	Unit	Source
gf	-188.44	kJ/mol	Joback Method
hf	-608.44	kJ/mol	Joback Method
hfus	50.59	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.148		Crippen Method
mcvol	223.630	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
tb	878.78	K	Joback Method
tc	1111.41	K	Joback Method
tf	307.90 ± 0.20	K	NIST Webbook
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.32	J/mol×K	878.78	Joback Method
cpg	723.46	J/mol×K	917.55	Joback Method
cpg	734.82	J/mol×K	956.32	Joback Method
cpg	745.55	J/mol×K	995.09	Joback Method
cpg	755.76	J/mol×K	1033.86	Joback Method
cpg	765.59	J/mol×K	1072.64	Joback Method
cpg	775.16	J/mol×K	1111.41	Joback Method
hfust	22.51	kJ/mol	305.80	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26399360&Units=SI
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

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