3,5-DINITROBENZOTRIFLUORIDE

Other names: Benzene, 1,3-dinitro-5-(trifluoromethyl)-
1,3-Dinitro-5-trifluoromethyl-benzene
«alpha»,«alpha»,«alpha»-trifluoro-3,5-dinitrotoluene
Inchi: InChI=1S/C7H3F3N2O4/c8-7(9,10)4-1-5(11(13)14)3-6(2-4)12(15)16/h1-3H
InchiKey: QZADIXWDDVQVKM-UHFFFAOYSA-N
Formula: C7H3F3N2O4
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])cc(C(F)(F)F)c1
Mol. weight [g/mol]: 236.10

Physical Properties

Property code	Value	Unit	Source
ea	1.99 ± 0.07	eV	NIST Webbook
hf	-553.58	kJ/mol	Cheméo Relay (1.0)
hfus	31.70	kJ/mol	Joback Method
hvap	71.55	kJ/mol	Cheméo Relay (1.0)
ie	11.00	eV	Cheméo Relay (1.0)
log10ws	-3.73		Cheméo Relay (1.0)
logp	2.522		Crippen Method
mcvol	125.880	ml/mol	McGowan Method
tb	507.22	K	Cheméo Relay (1.0)
tf	345.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.19	J/mol×K	694.46	Joback Method
cpg	335.46	J/mol×K	736.39	Joback Method
cpg	342.87	J/mol×K	778.31	Joback Method
cpg	349.50	J/mol×K	820.24	Joback Method
cpg	355.44	J/mol×K	862.16	Joback Method
cpg	360.75	J/mol×K	904.09	Joback Method
cpg	365.53	J/mol×K	946.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C401990&Units=SI
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
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point