

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
CAS:	401-99-0

Physical Properties

Property code	Value	Unit	Source
ea	1.99 ± 0.07	eV	NIST Webbook
gf	-409.28	kJ/mol	Joback Method
hf	-592.82	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	64.21	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.522		Crippen Method
mcvol	125.880	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	694.46	K	Joback Method
tc	946.01	K	Joback Method
tf	511.52	K	Joback Method
vc	0.526	m ³ /kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C401990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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

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