2-Trifluoromethyl-N,N-dimethyl-4-nitroaniline

Other names: N,N-Dimethyl-4-nitro-2-trifluoromethylaniline
Benzene, 1-trifluoromethyl-2-dimethylamino-5-nitro-
Inchi: InChI=1S/C9H9F3N2O2/c1-13(2)8-4-3-6(14(15)16)5-7(8)9(10,11)12/h3-5H,1-2H3
InchiKey: OIZCWRMHLSZGKT-UHFFFAOYSA-N
Formula: C9H9F3N2O2
SMILES: CN(C)c1ccc([N+](=O)[O-])cc1C(F)(F)F
Mol. weight [g/mol]: 234.18
CAS: 54672-09-2

Physical Properties

Property code	Value	Unit	Source
gf	-317.21	kJ/mol	Joback Method
hf	-555.81	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	54.11	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.680		Crippen Method
mcvol	146.620	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
tb	600.82	K	Joback Method
tc	817.56	K	Joback Method
tf	422.92	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.54	J/mol×K	600.82	Joback Method
cpg	385.68	J/mol×K	636.94	Joback Method
cpg	396.89	J/mol×K	673.07	Joback Method
cpg	407.22	J/mol×K	709.19	Joback Method
cpg	416.74	J/mol×K	745.31	Joback Method
cpg	425.50	J/mol×K	781.44	Joback Method
cpg	433.57	J/mol×K	817.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54672092&Units=SI

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
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