N,N-Dimethyl-4-nitro-3(trifluoromethyl)aniline

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

Physical Properties

Property code	Value	Unit	Source
hf	-567.93	kJ/mol	Cheméo Relay (1.0)
hfus	28.54	kJ/mol	Joback Method
ie	8.17	eV	Cheméo Relay (1.0)
logp	2.680		Crippen Method
mcvol	146.620	ml/mol	McGowan Method
tb	528.58	K	Cheméo Relay (1.0)
tf	329.79	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41512623&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point