4-Amino-3-nitrobenzotrifluoride

Other names:	2-Nitro-4-(trifluoromethyl)aniline
	4-Amino-3-nitrobenzotrifluoride
	4-Trifluoromethyl 2-nitroaniline
	Benzenamine, 2-nitro-4-(trifluoromethyl)-
	p-Toluidine, «alpha»,«alpha»,«alpha»-trifluoro-2-nitro-
	«alpha»,«alpha»,«alpha»-Trifluoro-2-nitro-p-toluidine
Inchi:	InChI=1S/C7H5F3N2O2/c8-7(9,10)4-1-2-5(11)6(3-4)12(13)14/h1-3H,11H2
InchiKey:	ATXBGHLILIABGX-UHFFFAOYSA-N
Formula:	C7H5F3N2O2
SMILES:	Nc1ccc(C(F)(F)F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	206.12

Physical Properties

Property code	Value	Unit	Source
hfus	25.53	kJ/mol	Joback Method
ie	9.05	eV	Cheméo Relay (1.0)
log10ws	-3.35		Cheméo Relay (1.0)
logp	2.196		Crippen Method
mcvol	118.440	ml/mol	McGowan Method
tb	529.08	K	Cheméo Relay (1.0)
tf	384.10	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.10	J/mol×K	615.15	Joback Method
cpg	307.46	J/mol×K	654.52	Joback Method
cpg	315.99	J/mol×K	693.88	Joback Method
cpg	323.75	J/mol×K	733.25	Joback Method
cpg	330.80	J/mol×K	772.62	Joback Method
cpg	337.20	J/mol×K	811.98	Joback Method
cpg	343.01	J/mol×K	851.35	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C400986&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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