4-Bromo-3-nitrobenzotrifluoride

Other names:	3-Nitro-4-bromobenzotrifluoride
	Benzene, 1-bromo-2-nitro-4-(trifluoromethyl)-
	Toluene, 4-bromo-3-nitro-alpha,alpha,alpha-trifluoro-
Inchi:	InChI=1S/C7H3BrF3NO2/c8-5-2-1-4(7(9,10)11)3-6(5)12(13)14/h1-3H
InchiKey:	PESPBNYBZVIGRO-UHFFFAOYSA-N
Formula:	C7H3BrF3NO2
SMILES:	O=[N+]([O-])c1cc(C(F)(F)F)ccc1Br
Mol. weight [g/mol]:	270.00
CAS:	349-03-1

Physical Properties

Property code	Value	Unit	Source
gf	-430.51	kJ/mol	Joback Method
hf	-555.73	kJ/mol	Joback Method
hfus	25.62	kJ/mol	Joback Method
hvap	54.05	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.376		Crippen Method
mcvol	125.960	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
tb	608.78	K	Joback Method
tc	850.63	K	Joback Method
tf	427.71	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.61	J/mol×K	608.78	Joback Method
cpg	287.06	J/mol×K	649.09	Joback Method
cpg	294.68	J/mol×K	689.40	Joback Method
cpg	301.55	J/mol×K	729.70	Joback Method
cpg	307.75	J/mol×K	770.01	Joback Method
cpg	313.34	J/mol×K	810.32	Joback Method

cpg	318.41	J/mol×K	850.63	Joback Method

Sources

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=C349031&Units=SI
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
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