

2-Bromo-5-nitrobenzotrifluoride

Other names:	Benzene, 1-bromo-4-nitro-2-(trifluoromethyl)-
Inchi:	InChI=1S/C7H3BrF3NO2/c8-6-2-1-4(12(13)14)3-5(6)7(9,10)11/h1-3H
InchiKey:	SXEQQBBOAMHOID-UHFFFAOYSA-N
Formula:	C7H3BrF3NO2
SMILES:	O=[N+]([O-])c1ccc(Br)c(C(F)(F)F)c1
Mol. weight [g/mol]:	270.00
CAS:	367-67-9

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	m ³ /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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.50 ± 0.50	K	0.40	NIST Webbook

Sources

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=C367679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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