Benzene, 1-bromo-3-(trifluoromethyl)-

Other names:	Toluene, m-bromo-«alpha»,«alpha»,«alpha»-trifluoro- m-(Trifluoromethyl)bromobenzene m-(Trifluoromethyl)phenyl bromide m-Bromo(trifluoromethyl)benzene m-Bromo-«alpha»,«alpha»,«alpha»-trifluorotoluene m-Bromobenzotrifluoride 1-Bromo-3-(trifluoromethyl)benzene 3-(Trifluoromethyl)bromobenzene 3-(Trifluoromethyl)phenyl bromide 3-Bromobenzotrifluoride 3-Bromobenzyltrifluoride Toluene, «alpha»,«alpha»,«alpha»-trifluoro-3-bromo- 3-Brombenzotrifluorid 3-Bromotrifluoromethylbenzene NSC 9468 3-bromo-«alpha»,«alpha»,«alpha»-trifluorotoluene
Inchi:	InChI=1S/C7H4BrF3/c8-6-3-1-2-5(4-6)7(9,10)11/h1-4H
InchiKey:	NNMBNYHMJRJUBC-UHFFFAOYSA-N
Formula:	C7H4BrF3
SMILES:	FC(F)(F)c1cccc(Br)c1
Mol. weight [g/mol]:	225.01
CAS:	401-78-5

Physical Properties

Property code	Value	Unit	Source
gf	-456.43	kJ/mol	Joback Method
hf	-533.50	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	36.80	kJ/mol	Joback Method
ie	9.36	eV	NIST Webbook
log10ws	-3.74		Crippen Method
logp	3.468		Crippen Method
mcvol	108.540	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	426.50 ± 0.50	K	NIST Webbook
tb	428.00	K	NIST Webbook
tb	424.70	K	NIST Webbook

tb	426.50 ± 0.50	K	NIST Webbook
tc	663.16	K	Joback Method
tf	271.58	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.47	J/mol×K	451.96	Joback Method
cpg	211.43	J/mol×K	487.16	Joback Method
cpg	220.58	J/mol×K	522.36	Joback Method
cpg	228.96	J/mol×K	557.56	Joback Method
cpg	236.64	J/mol×K	592.76	Joback Method
cpg	243.66	J/mol×K	627.96	Joback Method
cpg	250.07	J/mol×K	663.16	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=C401785&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
ie: Ionization energy
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