

Benzene, 4-bromo-1-chloro-2-(trifluoromethyl)-

Other names:	5-Bromo-2-chlorobenzotrifluoride Toluene, 5-bromo-2-chloro-«alpha», «alpha», «alpha»-trifluoro- 5-Bromo-2-chloro-«alpha», «alpha», «alpha»-trifluorotoluene 4-bromo-2-chloro-«alpha», «alpha», «alpha»-trifluorotoluene
Inchi:	InChI=1S/C7H3BrClF3/c8-4-1-2-6(9)5(3-4)7(10,11)12/h1-3H
InchiKey:	XGOCKBMEZPNDPJ-UHFFFAOYSA-N
Formula:	C7H3BrClF3
SMILES:	FC(F)(F)c1cc(Br)ccc1Cl
Mol. weight [g/mol]:	259.45
CAS:	445-01-2

Physical Properties

Property code	Value	Unit	Source
gf	-477.99	kJ/mol	Joback Method
hf	-560.71	kJ/mol	Joback Method
hfus	18.46	kJ/mol	Joback Method
hvap	41.85	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.121		Crippen Method
mcvol	120.780	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	467.00 ± 1.00	K	NIST Webbook
tc	712.90	K	Joback Method
tf	314.02	K	Joback Method
vc	0.473	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.98	J/mol×K	494.37	Joback Method
cpg	232.63	J/mol×K	530.79	Joback Method
cpg	240.54	J/mol×K	567.21	Joback Method
cpg	247.75	J/mol×K	603.63	Joback Method
cpg	254.32	J/mol×K	640.06	Joback Method

cpg	260.31	J/mol×K	676.48	Joback Method
cpg	265.75	J/mol×K	712.90	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=C445012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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