4-(Trifluoromethoxy)bromobenzene

Other names:	1-Bromo-4-(trifluoromethoxy)benzene
	Benzene, 1-bromo-4-(trifluoromethoxy)-
Inchi:	InChI=1S/C7H4BrF3O/c8-5-1-3-6(4-2-5)12-7(9,10)11/h1-4H
InchiKey:	SEAOBYFQWJFORM-UHFFFAOYSA-N
Formula:	C7H4BrF3O
SMILES:	FC(F)(F)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	241.01

Physical Properties

Property code	Value	Unit	Source
hfus	15.84	kJ/mol	Joback Method
hvap	46.44	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-3.75		Cheméo Relay (1.0)
logp	3.348		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
tb	437.15	K	Cheméo Relay (1.0)
tf	233.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.56	J/mol×K	474.38	Joback Method
cpg	232.14	J/mol×K	509.31	Joback Method
cpg	241.02	J/mol×K	544.23	Joback Method
cpg	249.24	J/mol×K	579.16	Joback Method
cpg	256.83	J/mol×K	614.08	Joback Method
cpg	263.82	J/mol×K	649.01	Joback Method
cpg	270.25	J/mol×K	683.93	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C407147&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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point