

3,5-Bis(trifluoromethyl)bromobenzene

Other names:	3,5-di(Trifluoromethyl)bromobenzene Benzene, 1-bromo-3,5-bis(trifluoromethyl)- m-Xylene, 5-bromo-alpha,alpha,alpha,alpha',alpha',alpha'-hexafluoro- 1-bromo-3,5-bis(trifluoromethyl)benzene
Inchi:	InChI=1S/C8H3BrF6/c9-6-2-4(7(10,11)12)1-5(3-6)8(13,14)15/h1-3H
InchiKey:	CSVCVIHEBDJTCJ-UHFFFAOYSA-N
Formula:	C8H3BrF6
SMILES:	FC(F)(F)c1cc(Br)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	293.00
CAS:	328-70-1

Physical Properties

Property code	Value	Unit	Source
gf	-1039.23	kJ/mol	Joback Method
hf	-1162.69	kJ/mol	Joback Method
hfus	18.68	kJ/mol	Joback Method
hvap	35.94	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.487		Crippen Method
mcvol	127.940	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
tb	427.20	K	NIST Webbook
tc	665.06	K	Joback Method
tf	299.56	K	Joback Method
vc	0.523	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.61	J/molxK	474.40	Joback Method
cpg	279.66	J/molxK	506.18	Joback Method
cpg	288.88	J/molxK	537.95	Joback Method
cpg	297.32	J/molxK	569.73	Joback Method
cpg	305.04	J/molxK	601.51	Joback Method

cpg	312.09	J/mol×K	633.29	Joback Method
cpg	318.52	J/mol×K	665.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C328701&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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