

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

Physical Properties

Property code	Value	Unit	Source
hfus	18.68	kJ/mol	Joback Method
ie	9.68	eV	Cheméo Relay (1.0)
log10ws	-5.09		Cheméo Relay (1.0)
logp	4.487		Crippen Method
mcvol	127.940	ml/mol	McGowan Method
tb	427.20	K	NIST Webbook
tf	361.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C328701&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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

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