2,4-Bis(trifluoromethyl)bromobenzene

Inchi: InChI=1S/C8H3BrF6/c9-6-2-1-4(7(10,11)12)3-5(6)8(13,14)15/h1-3H
InchiKey: QDEJWLIKRLJYEK-UHFFFAOYSA-N
Formula: C8H3BrF6
SMILES: FC(F)(F)c1ccc(Br)c(C(F)(F)F)c1
Mol. weight [g/mol]: 293.00
CAS: 327-75-3

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	474.40	K	Joback Method
tc	665.06	K	Joback Method
tf	299.56	K	Joback Method
vc	0.523	m3/kmol	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.20	K	98.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C327753&Units=SI
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume