

Benzene, 1-bromo-2,4,5-trifluoro-

Other names:	1-Bromo-2,4,5-trifluorobenzene 2-Bromo-1,4,5-trifluorobenzene
Inchi:	InChI=1S/C6H2BrF3/c7-3-1-5(9)6(10)2-4(3)8/h1-2H
InchiKey:	DVTULTINXNWGJY-UHFFFAOYSA-N
Formula:	C6H2BrF3
SMILES:	Fc1cc(F)c(Br)cc1F
Mol. weight [g/mol]:	210.98
CAS:	327-52-6

Physical Properties

Property code	Value	Unit	Source
gf	-486.95	kJ/mol	Joback Method
hf	-527.05	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	37.20	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.866		Crippen Method
mvol	94.450	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	442.27	K	Joback Method
tc	645.14	K	Joback Method
tf	282.93	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.19	J/molxK	442.27	Joback Method
cpg	167.83	J/molxK	476.08	Joback Method
cpg	174.10	J/molxK	509.89	Joback Method
cpg	180.01	J/molxK	543.70	Joback Method
cpg	185.57	J/molxK	577.51	Joback Method
cpg	190.79	J/molxK	611.33	Joback Method
cpg	195.70	J/molxK	645.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C327526&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
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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