2,3,6-Trifluorobenzylbromide

Inchi: InChI=1S/C7H4BrF3/c8-3-4-5(9)1-2-6(10)7(4)11/h1-2H,3H2
InchiKey: JPBWEVKHPSNBCE-UHFFFAOYSA-N
Formula: C7H4BrF3
SMILES: Fc1ccc(F)c(CBr)c1F
Mol. weight [g/mol]: 225.01
CAS: 151412-02-1

Physical Properties

Property code	Value	Unit	Source
gf	-478.53	kJ/mol	Joback Method
hf	-547.69	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	39.42	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.999		Crippen Method
mcvol	108.540	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
tb	465.15	K	Joback Method
tc	665.56	K	Joback Method
tf	294.20	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.44	J/mol×K	465.15	Joback Method
cpg	206.45	J/mol×K	498.55	Joback Method
cpg	214.02	J/mol×K	531.95	Joback Method
cpg	221.17	J/mol×K	565.36	Joback Method
cpg	227.91	J/mol×K	598.76	Joback Method
cpg	234.27	J/mol×K	632.16	Joback Method
cpg	240.24	J/mol×K	665.56	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C151412021&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