p-Bromophenyl trifluoromethyl ether

Other names: 1-Bromo-4-(trifluoromethoxy)benzene
Benzene, 1-bromo-4-(trifluoromethoxy)-
Inchi: InChI=1S/C7H4BrF3O/c8-5-1-3-6(4-2-5)12-7(9,10)11/h1-4H
InchiKey: SEAOBYFQWJFORM-UHFFFAOYSA-N
Formula: C7H4BrF3O
SMILES: FC(F)(F)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 241.00
CAS: 407-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-561.43	kJ/mol	Joback Method
hf	-665.72	kJ/mol	Joback Method
hfus	15.84	kJ/mol	Joback Method
hvap	39.21	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.348		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	474.38	K	Joback Method
tc	683.93	K	Joback Method
tf	293.81	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.56	J/mol×K	474.38	Joback Method
cpg	232.14	J/mol×K	509.31	Joback Method
cpg	241.02	J/mol×K	544.23	Joback Method
cpg	249.24	J/mol×K	579.16	Joback Method
cpg	256.83	J/mol×K	614.08	Joback Method
cpg	263.82	J/mol×K	649.01	Joback Method
cpg	270.25	J/mol×K	683.93	Joback Method

Sources

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=C407147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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