Bromodifluoroacetylchloride

Inchi: InChI=1S/C2BrClF2O/c3-2(5,6)1(4)7
InchiKey: LYJKGSALBRSKNL-UHFFFAOYSA-N
Formula: C2BrClF2O
SMILES: O=C(Cl)C(F)(F)Br
Mol. weight [g/mol]: 193.38
CAS: 3832-48-2

Physical Properties

Property code	Value	Unit	Source
gf	-547.35	kJ/mol	Joback Method
hf	-587.57	kJ/mol	Joback Method
hfus	10.76	kJ/mol	Joback Method
hvap	34.68	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.740		Crippen Method
mcvol	73.890	ml/mol	McGowan Method
pc	5205.63	kPa	Joback Method
tb	397.93	K	Joback Method
tc	599.93	K	Joback Method
tf	255.55	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	111.30	J/mol×K	397.93	Joback Method
cpg	115.55	J/mol×K	431.60	Joback Method
cpg	119.36	J/mol×K	465.26	Joback Method
cpg	122.76	J/mol×K	498.93	Joback Method
cpg	125.78	J/mol×K	532.59	Joback Method
cpg	128.45	J/mol×K	566.26	Joback Method
cpg	130.79	J/mol×K	599.93	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=C3832482&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