1-Bromo-3,3,3-trifluoroacetone

Other names:	3-Bromo-1,1,1-trifluoropropanone
	3-Bromo-1,1,1-trifluoro-2-propanone
	2-Propanone, 3-bromo-1,1,1-trifluoro-
	3-Bromo-1,1,1-trifluoroacetone
Inchi:	InChI=1S/C3H2BrF3O/c4-1-2(8)3(5,6)7/h1H2
InchiKey:	ONZQYZKCUHFORE-UHFFFAOYSA-N
Formula:	C3H2BrF3O
SMILES:	O=C(CBr)C(F)(F)F
Mol. weight [g/mol]:	190.95
CAS:	431-35-6

Physical Properties

Property code	Value	Unit	Source
gf	-721.81	kJ/mol	Joback Method
hf	-788.58	kJ/mol	Joback Method
hfus	12.24	kJ/mol	Joback Method
hvap	31.71	kJ/mol	Joback Method
ie	10.92 ± 0.02	eV	NIST Webbook
log10ws	-1.45		Crippen Method
logp	1.513		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	359.00 ± 1.00	K	NIST Webbook
tc	564.21	K	Joback Method
tf	237.49	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.87	J/mol×K	382.65	Joback Method
cpg	138.83	J/mol×K	412.91	Joback Method
cpg	144.36	J/mol×K	443.17	Joback Method
cpg	149.46	J/mol×K	473.43	Joback Method

cpg	154.17	J/mol×K	503.69	Joback Method
cpg	158.51	J/mol×K	533.95	Joback Method
cpg	162.49	J/mol×K	564.21	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=C431356&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
ie:	Ionization energy
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