2-Propanone, 1-bromo-1,1,3-trichloro-

Inchi: InChI=1S/C3H2BrCl3O/c4-3(6,7)2(8)1-5/h1H2
InchiKey: LZGRQTQVHSDAQR-UHFFFAOYSA-N
Formula: C3H2BrCl3O
SMILES: O=C(CCl)C(Cl)(Cl)Br
Mol. weight [g/mol]: 240.31
CAS: 16995-36-1

Physical Properties

Property code	Value	Unit	Source
gf	-173.17	kJ/mol	Joback Method
hf	-247.47	kJ/mol	Joback Method
hfus	15.59	kJ/mol	Joback Method
hvap	47.31	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.321		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	497.13	K	Joback Method
tc	734.47	K	Joback Method
tf	325.48	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.41	J/mol×K	497.13	Joback Method
cpg	183.82	J/mol×K	694.91	Joback Method
cpg	180.89	J/mol×K	655.36	Joback Method
cpg	177.53	J/mol×K	615.80	Joback Method
cpg	173.70	J/mol×K	576.24	Joback Method
cpg	169.35	J/mol×K	536.69	Joback Method
cpg	186.40	J/mol×K	734.47	Joback Method
dvisc	0.0004696	Pa×s	497.13	Joback Method
dvisc	0.0005915	Pa×s	468.52	Joback Method

dvisc	0.0007677	Pa×s	439.91	Joback Method
dvisc	0.0010331	Pa×s	411.31	Joback Method
dvisc	0.0014535	Pa×s	382.70	Joback Method
dvisc	0.0021610	Pa×s	354.09	Joback Method
dvisc	0.0034447	Pa×s	325.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16995361&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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