2,2,3-trichloropropanal

Inchi: InChI=1S/C3H3Cl3O/c4-1-3(5,6)2-7/h2H,1H2
InchiKey: VMVQOWJGWBIGEU-UHFFFAOYSA-N
Formula: C3H3Cl3O
SMILES: O=CC(Cl)(Cl)CCl
Mol. weight [g/mol]: 161.41
CAS: 7789-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-158.09	kJ/mol	Joback Method
hf	-246.80	kJ/mol	Joback Method
hfus	10.99	kJ/mol	Joback Method
hvap	40.85	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.598		Crippen Method
mcvol	91.420	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	425.76	K	Joback Method
tc	638.66	K	Joback Method
tf	223.60 ± 0.60	K	NIST Webbook
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.23	J/mol×K	425.76	Joback Method
cpg	148.81	J/mol×K	461.24	Joback Method
cpg	153.88	J/mol×K	496.73	Joback Method
cpg	158.49	J/mol×K	532.21	Joback Method
cpg	162.66	J/mol×K	567.69	Joback Method
cpg	166.44	J/mol×K	603.17	Joback Method
cpg	169.85	J/mol×K	638.66	Joback Method
dvisc	0.0055718	Pa×s	257.75	Joback Method
dvisc	0.0031025	Pa×s	285.75	Joback Method

dvisc	0.0019179	Pa×s	313.75	Joback Method
dvisc	0.0012828	Pa×s	341.75	Joback Method
dvisc	0.0009119	Pa×s	369.76	Joback Method
dvisc	0.0006801	Pa×s	397.76	Joback Method
dvisc	0.0005272	Pa×s	425.76	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=C7789904&Units=SI

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