chloromethyl trichloroacetate

Inchi: InChI=1S/C3H2Cl4O2/c4-1-9-2(8)3(5,6)7/h1H2
InchiKey: JUBDPPCRYPFPIX-UHFFFAOYSA-N
Formula: C3H2Cl4O2
SMILES: O=C(OCCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 211.86

Physical Properties

Property code	Value	Unit	Source
gf	-304.42	kJ/mol	Joback Method
hf	-421.76	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	47.67	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.096		Crippen Method
mcvol	109.530	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
rinpol	1031.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1038.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1654.00		NIST Webbook
tb	490.82	K	Joback Method
tc	714.30	K	Joback Method
tf	317.83	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.92	J/mol×K	490.82	Joback Method

cpg	198.16	J/mol×K	677.05	Joback Method
cpg	194.68	J/mol×K	639.81	Joback Method
cpg	190.84	J/mol×K	602.56	Joback Method
cpg	186.61	J/mol×K	565.31	Joback Method
cpg	181.98	J/mol×K	528.07	Joback Method
cpg	201.29	J/mol×K	714.30	Joback Method
dvisc	0.0003762	Pa×s	490.82	Joback Method
dvisc	0.0004782	Pa×s	461.99	Joback Method
dvisc	0.0006276	Pa×s	433.16	Joback Method
dvisc	0.0008562	Pa×s	404.33	Joback Method
dvisc	0.0012252	Pa×s	375.49	Joback Method
dvisc	0.0018609	Pa×s	346.66	Joback Method
dvisc	0.0030492	Pa×s	317.83	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=R112644&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume