7-chloroheptyl chloroacetate

Other names: 1-Heptanol, 7-chloro, chloroacetate
Inchi: InChI=1S/C9H16Cl2O2/c10-6-4-2-1-3-5-7-13-9(12)8-11/h1-8H2
InchiKey: WXIUUGACTTYPLC-UHFFFAOYSA-N
Formula: C9H16Cl2O2
SMILES: O=C(CCl)OCCCCCCCCl
Mol. weight [g/mol]: 227.13

Physical Properties

Property code	Value	Unit	Source
gf	-232.88	kJ/mol	Joback Method
hf	-505.37	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.958		Crippen Method
mcvol	169.590	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1559.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1559.00		NIST Webbook
ripol	2333.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2308.00		NIST Webbook
tb	556.47	K	Joback Method
tc	740.45	K	Joback Method
tf	323.19	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.98	J/mol×K	556.47	Joback Method

cpg	435.85	J/mol×K	709.79	Joback Method
cpg	425.73	J/mol×K	679.13	Joback Method
cpg	415.09	J/mol×K	648.46	Joback Method
cpg	403.92	J/mol×K	617.80	Joback Method
cpg	392.22	J/mol×K	587.13	Joback Method
cpg	445.47	J/mol×K	740.45	Joback Method
dvisc	0.0002308	Pa×s	556.47	Joback Method
dvisc	0.0002970	Pa×s	517.59	Joback Method
dvisc	0.0003982	Pa×s	478.71	Joback Method
dvisc	0.0005623	Pa×s	439.83	Joback Method
dvisc	0.0008489	Pa×s	400.95	Joback Method
dvisc	0.0014003	Pa×s	362.07	Joback Method
dvisc	0.0026055	Pa×s	323.19	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=R111834&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
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