CHLOROMETHYL 2-CHLOROHEPTANOATE

Other names: 2-Chloroheptanoic acid, chloromethyl ester
Inchi: InChI=1S/C8H14Cl2O2/c1-2-3-4-5-7(10)8(11)12-6-9/h7H,2-6H2,1H3
InchiKey: OEONOJHNBIZMIO-UHFFFAOYSA-N
Formula: C8H14Cl2O2
SMILES: CCCCCC(Cl)C(=O)OCCl
Mol. weight [g/mol]: 213.10

Physical Properties

Property code	Value	Unit	Source
hf	-586.90	kJ/mol	Cheméo Relay (1.0)
hfus	24.13	kJ/mol	Joback Method
hvap	59.32	kJ/mol	Cheméo Relay (1.0)
logp	2.914		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
rinpol	1316.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1328.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	493.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.71	J/mol×K	533.15	Joback Method
cpg	396.95	J/mol×K	722.96	Joback Method
cpg	387.84	J/mol×K	691.33	Joback Method
cpg	378.23	J/mol×K	659.69	Joback Method
cpg	368.12	J/mol×K	628.06	Joback Method
cpg	357.50	J/mol×K	596.42	Joback Method
cpg	346.37	J/mol×K	564.79	Joback Method

dvisc	0.0006335	Pa×s	415.03	Joback Method
dvisc	0.0002408	Pa×s	533.15	Joback Method
dvisc	0.0003157	Pa×s	493.78	Joback Method
dvisc	0.0004339	Pa×s	454.41	Joback Method
dvisc	0.0035993	Pa×s	296.92	Joback Method
dvisc	0.0010012	Pa×s	375.66	Joback Method
dvisc	0.0017614	Pa×s	336.29	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418582&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature