CHLOROMETHYL 10-CHLORODODECANOATE

Other names: 10-Chlorododecanoic acid, chloromethyl ester
Inchi: InChI=1S/C13H24Cl2O2/c1-2-12(15)9-7-5-3-4-6-8-10-13(16)17-11-14/h12H,2-11H2,1H3
InchiKey: CKRGKKRODIRREL-UHFFFAOYSA-N
Formula: C13H24Cl2O2
SMILES: CCC(Cl)CCCCCCCCC(=O)OCCl
Mol. weight [g/mol]: 283.24

Physical Properties

Property code	Value	Unit	Source
hf	-696.47	kJ/mol	Cheméo Relay (1.0)
hfus	37.08	kJ/mol	Joback Method
hvap	82.21	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.24		Cheméo Relay (1.0)
logp	4.864		Crippen Method
mcvol	225.950	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1895.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1895.00		NIST Webbook
ripol	2480.00		NIST Webbook
ripol	2506.00		NIST Webbook
ripol	2512.00		NIST Webbook
ripol	2480.00		NIST Webbook
tb	575.07	K	Cheméo Relay (1.0)
tc	768.68	K	Cheméo Relay (1.0)
tf	277.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.55	J/mol×K	647.55	Joback Method
cpg	594.71	J/mol×K	677.68	Joback Method

cpg	609.14	J/mol×K	707.81	Joback Method
cpg	622.86	J/mol×K	737.94	Joback Method
cpg	635.88	J/mol×K	768.06	Joback Method
cpg	648.22	J/mol×K	798.19	Joback Method
cpg	659.91	J/mol×K	828.32	Joback Method
dvisc	0.0025326	Pa×s	353.27	Joback Method
dvisc	0.0011518	Pa×s	402.32	Joback Method
dvisc	0.0006217	Pa×s	451.36	Joback Method
dvisc	0.0003786	Pa×s	500.41	Joback Method
dvisc	0.0002520	Pa×s	549.46	Joback Method
dvisc	0.0001792	Pa×s	598.50	Joback Method
dvisc	0.0001343	Pa×s	647.55	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80419063&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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