CHLOROMETHYL 6-CHLOROUNDECANOATE

Other names: 6-Chloroundecanoic acid, chloromethyl ester
Inchi: InChI=1S/C12H22Cl2O2/c1-2-3-4-7-11(14)8-5-6-9-12(15)16-10-13/h11H,2-10H2,1H3
InchiKey: NHURGYSRXYAHKJ-UHFFFAOYSA-N
Formula: C12H22Cl2O2
SMILES: CCCCCC(Cl)CCCCC(=O)OCCl
Mol. weight [g/mol]: 269.21

Physical Properties

Property code	Value	Unit	Source
hf	-666.04	kJ/mol	Cheméo Relay (1.0)
hfus	34.49	kJ/mol	Joback Method
hvap	77.26	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.79		Cheméo Relay (1.0)
logp	4.474		Crippen Method
mcvol	211.860	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1783.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2369.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2350.00		NIST Webbook
tb	562.61	K	Cheméo Relay (1.0)
tc	752.74	K	Cheméo Relay (1.0)
tf	262.93	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.44	J/mol×K	624.67	Joback Method
cpg	542.05	J/mol×K	655.01	Joback Method
cpg	555.97	J/mol×K	685.35	Joback Method

cpg	569.22	J/mol×K	715.70	Joback Method
cpg	581.80	J/mol×K	746.04	Joback Method
cpg	593.73	J/mol×K	776.38	Joback Method
cpg	605.03	J/mol×K	806.72	Joback Method
dvisc	0.0027597	Pa×s	342.00	Joback Method
dvisc	0.0012714	Pa×s	389.11	Joback Method
dvisc	0.0006925	Pa×s	436.22	Joback Method
dvisc	0.0004246	Pa×s	483.33	Joback Method
dvisc	0.0002840	Pa×s	530.45	Joback Method
dvisc	0.0002028	Pa×s	577.56	Joback Method
dvisc	0.0001524	Pa×s	624.67	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418924&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

Cheméo Relay (1.0):

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