Chloromethyl dodecanoate

Other names: Dodecanoic acid, chloromethyl ester
Inchi: InChI=1S/C13H25ClO2/c1-2-3-4-5-6-7-8-9-10-11-13(15)16-12-14/h2-12H2,1H3
InchiKey: XCHDYWCWXAASER-UHFFFAOYSA-N
Formula: C13H25ClO2
SMILES: CCCCCCCCCCCC(=O)OCCl
Mol. weight [g/mol]: 248.79
CAS: 61413-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-187.27	kJ/mol	Joback Method
hf	-572.19	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.647		Crippen Method
mcvol	213.710	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1694.00		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2087.00		NIST Webbook
ripol	2102.00		NIST Webbook
tb	610.56	K	Joback Method
tc	784.07	K	Joback Method
tf	338.35	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.83	J/mol×K	610.56	Joback Method

cpg	563.46	J/mol×K	639.48	Joback Method
cpg	578.43	J/mol×K	668.40	Joback Method
cpg	592.72	J/mol×K	697.32	Joback Method
cpg	606.37	J/mol×K	726.24	Joback Method
cpg	619.38	J/mol×K	755.15	Joback Method
cpg	631.77	J/mol×K	784.07	Joback Method
dvisc	0.0024461	Pa×s	338.35	Joback Method
dvisc	0.0011849	Pa×s	383.72	Joback Method
dvisc	0.0006691	Pa×s	429.09	Joback Method
dvisc	0.0004215	Pa×s	474.45	Joback Method
dvisc	0.0002878	Pa×s	519.82	Joback Method
dvisc	0.0002089	Pa×s	565.19	Joback Method
dvisc	0.0001590	Pa×s	610.56	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=C61413670&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