Dodecyl 3-chlorobutanoate

Other names: Butanoic acid, 3-chloro, dodecyl ester
Inchi: InChI=1S/C16H31ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-19-16(18)14-15(2)17/h15H,3-14H2
InchiKey: AUFXSBSHIKABLE-UHFFFAOYSA-N
Formula: C16H31ClO2
SMILES: CCCCCCCCCCCCOC(=O)CC(C)Cl
Mol. weight [g/mol]: 290.87

Physical Properties

Property code	Value	Unit	Source
gf	-164.45	kJ/mol	Joback Method
hf	-639.39	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.468		Crippen Method
mcvol	255.980	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	1938.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1929.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	678.76	K	Joback Method
tc	853.20	K	Joback Method
tf	357.16	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.02	J/mol×K	678.76	Joback Method

cpg	728.39	J/mol×K	707.83	Joback Method
cpg	744.94	J/mol×K	736.91	Joback Method
cpg	760.71	J/mol×K	765.98	Joback Method
cpg	775.70	J/mol×K	795.05	Joback Method
cpg	789.95	J/mol×K	824.12	Joback Method
cpg	803.46	J/mol×K	853.20	Joback Method
dvisc	0.0024442	Pa×s	357.16	Joback Method
dvisc	0.0010191	Pa×s	410.76	Joback Method
dvisc	0.0005200	Pa×s	464.36	Joback Method
dvisc	0.0003050	Pa×s	517.96	Joback Method
dvisc	0.0001977	Pa×s	571.56	Joback Method
dvisc	0.0001380	Pa×s	625.16	Joback Method
dvisc	0.0001020	Pa×s	678.76	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=R28166&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume