Dodecyl 4-chlorobutanoate

Other names: Butanoic acid, 4-chloro, dodecyl ester
Inchi: InChI=1S/C16H31ClO2/c1-2-3-4-5-6-7-8-9-10-11-15-19-16(18)13-12-14-17/h2-15H2,1H3
InchiKey: AMCRHNDYMZXQRU-UHFFFAOYSA-N
Formula: C16H31ClO2
SMILES: CCCCCCCCCCCCOC(=O)CCCCl
Mol. weight [g/mol]: 290.87

Physical Properties

Property code	Value	Unit	Source
gf	-162.01	kJ/mol	Joback Method
hf	-634.11	kJ/mol	Joback Method
hfus	44.18	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.470		Crippen Method
mcvol	255.980	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2016.00		NIST Webbook
rinpol	2014.00		NIST Webbook
rinpol	2016.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	2001.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	679.20	K	Joback Method
tc	851.53	K	Joback Method
tf	372.16	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.59	J/mol×K	679.20	Joback Method

cpg	727.71	J/mol×K	707.92	Joback Method
cpg	744.05	J/mol×K	736.64	Joback Method
cpg	759.63	J/mol×K	765.36	Joback Method
cpg	774.47	J/mol×K	794.09	Joback Method
cpg	788.57	J/mol×K	822.81	Joback Method
cpg	801.97	J/mol×K	851.53	Joback Method
dvisc	0.0019268	Pa×s	372.16	Joback Method
dvisc	0.0008962	Pa×s	423.33	Joback Method
dvisc	0.0004917	Pa×s	474.51	Joback Method
dvisc	0.0003032	Pa×s	525.68	Joback Method
dvisc	0.0002037	Pa×s	576.85	Joback Method
dvisc	0.0001460	Pa×s	628.03	Joback Method
dvisc	0.0001101	Pa×s	679.20	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=R28170&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