Hexyl 4-chlorobutanoate

Other names: Butanoic acid, 4-chloro, hexyl ester
Inchi: InChI=1S/C10H19ClO2/c1-2-3-4-5-9-13-10(12)7-6-8-11/h2-9H2,1H3
InchiKey: NJJCFVMCDUBLGH-UHFFFAOYSA-N
Formula: C10H19ClO2
SMILES: CCCCCCOC(=O)CCCCl
Mol. weight [g/mol]: 206.71

Physical Properties

Property code	Value	Unit	Source
gf	-212.53	kJ/mol	Joback Method
hf	-510.27	kJ/mol	Joback Method
hfus	28.64	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.129		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1401.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1409.00		NIST Webbook
tb	541.92	K	Joback Method
tc	719.34	K	Joback Method
tf	304.54	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.46	J/mol×K	541.92	Joback Method

cpg	412.10	J/mol×K	571.49	Joback Method
cpg	425.18	J/mol×K	601.06	Joback Method
cpg	437.70	J/mol×K	630.63	Joback Method
cpg	449.68	J/mol×K	660.20	Joback Method
cpg	461.13	J/mol×K	689.77	Joback Method
cpg	472.05	J/mol×K	719.34	Joback Method
dvisc	0.0028840	Pa×s	304.54	Joback Method
dvisc	0.0014664	Pa×s	344.10	Joback Method
dvisc	0.0008572	Pa×s	383.67	Joback Method
dvisc	0.0005540	Pa×s	423.23	Joback Method
dvisc	0.0003858	Pa×s	462.79	Joback Method
dvisc	0.0002844	Pa×s	502.36	Joback Method
dvisc	0.0002192	Pa×s	541.92	Joback Method

Sources

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=R28287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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