

Hexyl 2-chlorobutanoate

Other names:	Butanoic acid, 2-chloro, hexyl ester
Inchi:	InChI=1S/C10H19ClO2/c1-3-5-6-7-8-13-10(12)9(11)4-2/h9H,3-8H2,1-2H3
InchiKey:	GAONBEAFOOASRD-UHFFFAOYSA-N
Formula:	C10H19ClO2
SMILES:	CCCCCCOC(=O)C(Cl)CC
Mol. weight [g/mol]:	206.71

Physical Properties

Property code	Value	Unit	Source
gf	-214.97	kJ/mol	Joback Method
hf	-515.55	kJ/mol	Joback Method
hfus	25.12	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.127		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1327.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1330.00		NIST Webbook
tb	541.48	K	Joback Method
tc	722.34	K	Joback Method
tf	289.54	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.76	J/molxK	541.48	Joback Method
cpg	462.76	J/molxK	692.19	Joback Method
cpg	451.10	J/molxK	662.05	Joback Method
cpg	438.88	J/molxK	631.91	Joback Method

cpg	426.09	J/molxK	601.77	Joback Method
cpg	412.72	J/molxK	571.62	Joback Method
cpg	473.86	J/molxK	722.34	Joback Method
dvisc	0.0002061	Paxs	541.48	Joback Method
dvisc	0.0002738	Paxs	499.49	Joback Method
dvisc	0.0003832	Paxs	457.50	Joback Method
dvisc	0.0005741	Paxs	415.51	Joback Method
dvisc	0.0009417	Paxs	373.52	Joback Method
dvisc	0.0017512	Paxs	331.53	Joback Method
dvisc	0.0038985	Paxs	289.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28269&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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