Heptyl 2-chlorobutanoate

Other names: Butanoic acid, 2-chloro, heptyl ester
Inchi: InChI=1S/C11H21ClO2/c1-3-5-6-7-8-9-14-11(13)10(12)4-2/h10H,3-9H2,1-2H3
InchiKey: SLAXIYNQTGZROJ-UHFFFAOYSA-N
Formula: C11H21ClO2
SMILES: CCCCCCCOC(=O)C(Cl)CC
Mol. weight [g/mol]: 220.74

Physical Properties

Property code	Value	Unit	Source
gf	-206.55	kJ/mol	Joback Method
hf	-536.19	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.517		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1412.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1427.00		NIST Webbook
tb	564.36	K	Joback Method
tc	743.50	K	Joback Method
tf	300.81	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.93	J/mol×K	564.36	Joback Method
cpg	514.22	J/mol×K	713.64	Joback Method
cpg	501.98	J/mol×K	683.78	Joback Method
cpg	489.15	J/mol×K	653.93	Joback Method

cpg	475.70	J/mol×K	624.07	Joback Method
cpg	461.63	J/mol×K	594.22	Joback Method
cpg	525.87	J/mol×K	743.50	Joback Method
dvisc	0.0001859	Pa×s	564.36	Joback Method
dvisc	0.0002478	Pa×s	520.44	Joback Method
dvisc	0.0003484	Pa×s	476.51	Joback Method
dvisc	0.0005249	Pa×s	432.59	Joback Method
dvisc	0.0008677	Pa×s	388.66	Joback Method
dvisc	0.0016303	Pa×s	344.74	Joback Method
dvisc	0.0036823	Pa×s	300.81	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R28205&Units=SI

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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