Butanoic acid, 3-chloro, heptyl ester

Other names: Heptyl 3-chlorobutanoate
Inchi: InChI=1S/C11H21ClO2/c1-3-4-5-6-7-8-14-11(13)9-10(2)12/h10H,3-9H2,1-2H3
InchiKey: IVSMBZGOSOEERU-UHFFFAOYSA-N
Formula: C11H21ClO2
SMILES: CCCCCCCOC(=O)CC(C)Cl
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	1443.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1425.00		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	461.63	J/mol×K	594.22	Joback Method
cpg	475.70	J/mol×K	624.07	Joback Method
cpg	489.15	J/mol×K	653.93	Joback Method
cpg	501.98	J/mol×K	683.78	Joback Method
cpg	514.22	J/mol×K	713.64	Joback Method
cpg	525.87	J/mol×K	743.50	Joback Method
dvisc	0.0036823	Pa×s	300.81	Joback Method
dvisc	0.0016303	Pa×s	344.74	Joback Method
dvisc	0.0008677	Pa×s	388.66	Joback Method
dvisc	0.0005249	Pa×s	432.59	Joback Method
dvisc	0.0003484	Pa×s	476.51	Joback Method
dvisc	0.0002478	Pa×s	520.44	Joback Method
dvisc	0.0001859	Pa×s	564.36	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=R28219&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