

5-Chlorohexanoic acid, methyl ester

Inchi:	InChI=1S/C7H13ClO2/c1-6(8)4-3-5-7(9)10-2/h6H,3-5H2,1-2H3
InchiKey:	JFDGPJPDWIHCSL-UHFFFAOYSA-N
Formula:	C7H13ClO2
SMILES:	COC(=O)CCCC(C)Cl
Mol. weight [g/mol]:	164.63

Physical Properties

Property code	Value	Unit	Source
gf	-240.23	kJ/mol	Joback Method
hf	-453.63	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.957		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1615.00		NIST Webbook
tb	472.84	K	Joback Method
tc	659.46	K	Joback Method
tf	255.73	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.41	J/molxK	472.84	Joback Method
cpg	316.63	J/molxK	628.35	Joback Method
cpg	307.25	J/molxK	597.25	Joback Method
cpg	297.44	J/molxK	566.15	Joback Method
cpg	287.19	J/molxK	535.05	Joback Method
cpg	276.52	J/molxK	503.94	Joback Method

cpg	325.59	J/molxK	659.46	Joback Method
dvisc	0.0002680	Paxs	472.84	Joback Method
dvisc	0.0003514	Paxs	436.65	Joback Method
dvisc	0.0004840	Paxs	400.47	Joback Method
dvisc	0.0007104	Paxs	364.28	Joback Method
dvisc	0.0011348	Paxs	328.10	Joback Method
dvisc	0.0020358	Paxs	291.92	Joback Method
dvisc	0.0043091	Paxs	255.73	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=R309521&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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