

6-Chlorohexanoic acid, methyl ester

Other names:	methyl 6-chlorohexanoate
Inchi:	InChI=1S/C7H13ClO2/c1-10-7(9)5-3-2-4-6-8/h2-6H2,1H3
InchiKey:	RZYHYFOTLPEKJO-UHFFFAOYSA-N
Formula:	C7H13ClO2
SMILES:	COC(=O)CCCCCCl
Mol. weight [g/mol]:	164.63
CAS:	14273-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-237.79	kJ/mol	Joback Method
hf	-448.35	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.959		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1139.00		NIST Webbook
rinpol	1152.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1659.00		NIST Webbook
tb	473.28	K	Joback Method
tc	655.90	K	Joback Method
tf	270.73	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.22	J/molxK	473.28	Joback Method
cpg	276.01	J/molxK	503.72	Joback Method
cpg	286.40	J/molxK	534.15	Joback Method

cpg	296.38	J/molxK	564.59	Joback Method
cpg	305.96	J/molxK	595.03	Joback Method
cpg	315.13	J/molxK	625.46	Joback Method
cpg	323.90	J/molxK	655.90	Joback Method
dvisc	0.0030645	Paxs	270.73	Joback Method
dvisc	0.0016518	Paxs	304.49	Joback Method
dvisc	0.0010072	Paxs	338.25	Joback Method
dvisc	0.0006719	Paxs	372.00	Joback Method
dvisc	0.0004794	Paxs	405.76	Joback Method
dvisc	0.0003603	Paxs	439.52	Joback Method
dvisc	0.0002820	Paxs	473.28	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=C14273893&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/27-878-8/6-Chlorohexanoic-acid-methyl-ester.pdf>

Generated by Cheméo on 2024-04-30 14:37:10.456431676 +0000 UTC m=+16777079.377008988.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.