

6-Chlorohexanoic acid, 4-methoxy-2-methylbutyl ester

Inchi:	InChI=1S/C12H23ClO3/c1-11(7-9-15-2)10-16-12(14)6-4-3-5-8-13/h11H,3-10H2,1-2H3
InchiKey:	LGSOBKQSTTXLJH-UHFFFAOYSA-N
Formula:	C12H23ClO3
SMILES:	COCCC(C)COC(=O)CCCCCl
Mol. weight [g/mol]:	250.76

Physical Properties

Property code	Value	Unit	Source
gf	-303.13	kJ/mol	Joback Method
hf	-689.05	kJ/mol	Joback Method
hfus	31.49	kJ/mol	Joback Method
hvap	57.87	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	3.001		Crippen Method
mcvol	205.490	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1764.00		NIST Webbook
tb	609.66	K	Joback Method
tc	786.71	K	Joback Method
tf	334.31	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.28	J/molxK	609.66	Joback Method
cpg	539.41	J/molxK	639.17	Joback Method
cpg	553.90	J/molxK	668.68	Joback Method
cpg	567.75	J/molxK	698.19	Joback Method
cpg	580.95	J/molxK	727.70	Joback Method
cpg	593.52	J/molxK	757.20	Joback Method
cpg	605.46	J/molxK	786.71	Joback Method
dvisc	0.0023446	Paxs	334.31	Joback Method
dvisc	0.0010828	Paxs	380.20	Joback Method

dvisc	0.0005906	Paxs	426.09	Joback Method
dvisc	0.0003624	Paxs	471.99	Joback Method
dvisc	0.0002425	Paxs	517.88	Joback Method
dvisc	0.0001732	Paxs	563.77	Joback Method
dvisc	0.0001302	Paxs	609.66	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=U354729&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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