6-Chlorohexanoic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C13H17ClO3/c1-16-11-6-8-12(9-7-11)17-13(15)5-3-2-4-10-14/h6-9H,2-5,10H2
InchiKey: WIUNAWMQMZCBAR-UHFFFAOYSA-N
Formula: C13H17ClO3
SMILES: COc1ccc(OC(=O)CCCCCCl)cc1
Mol. weight [g/mol]: 256.73

Physical Properties

Property code	Value	Unit	Source
gf	-189.49	kJ/mol	Joback Method
hf	-479.35	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	63.42	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.400		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	664.64	K	Joback Method
tc	870.26	K	Joback Method
tf	399.52	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.37	J/mol×K	664.64	Joback Method
cpg	560.79	J/mol×K	835.99	Joback Method
cpg	549.74	J/mol×K	801.72	Joback Method
cpg	537.89	J/mol×K	767.45	Joback Method
cpg	525.21	J/mol×K	733.18	Joback Method
cpg	511.71	J/mol×K	698.91	Joback Method
cpg	571.04	J/mol×K	870.26	Joback Method
dvisc	0.0001221	Pa×s	664.64	Joback Method

dvisc	0.0001542	Pa×s	620.45	Joback Method
dvisc	0.0002019	Pa×s	576.27	Joback Method
dvisc	0.0002763	Pa×s	532.08	Joback Method
dvisc	0.0004004	Pa×s	487.89	Joback Method
dvisc	0.0006245	Pa×s	443.71	Joback Method
dvisc	0.0010749	Pa×s	399.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307622&Units=SI
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

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