

6-Chlorohexanoic acid, 3-methylphenyl ester

Inchi:	InChI=1S/C13H17ClO2/c1-11-6-5-7-12(10-11)16-13(15)8-3-2-4-9-14/h5-7,10H,2-4,8-9H2
InchiKey:	ZRXIFYCSKIEIGD-UHFFFAOYSA-N
Formula:	C13H17ClO2
SMILES:	<chem>Cc1cccc(OC(=O)CCCCCCl)c1</chem>
Mol. weight [g/mol]:	240.73

Physical Properties

Property code	Value	Unit	Source
gf	-84.49	kJ/mol	Joback Method
hf	-347.13	kJ/mol	Joback Method
hfus	30.06	kJ/mol	Joback Method
hvap	61.01	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.700		Crippen Method
mvol	189.950	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1803.00		NIST Webbook
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tb	642.22	K	Joback Method
tc	849.84	K	Joback Method
tf	377.29	K	Joback Method
vc	0.729	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.36	J/molxK	642.22	Joback Method
cpg	485.98	J/molxK	676.82	Joback Method
cpg	499.75	J/molxK	711.43	Joback Method
cpg	512.68	J/molxK	746.03	Joback Method
cpg	524.81	J/molxK	780.63	Joback Method
cpg	536.14	J/molxK	815.23	Joback Method
cpg	546.71	J/molxK	849.84	Joback Method
dvisc	0.0014793	Paxs	377.29	Joback Method

dvisc	0.0008357	Paxs	421.45	Joback Method
dvisc	0.0005262	Paxs	465.60	Joback Method
dvisc	0.0003589	Paxs	509.75	Joback Method
dvisc	0.0002602	Paxs	553.91	Joback Method
dvisc	0.0001978	Paxs	598.07	Joback Method
dvisc	0.0001562	Paxs	642.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U307621&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

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