3-Chlorobenzoic acid, 6-chlorohexyl ester

Inchi: InChI=1S/C13H16Cl2O2/c14-8-3-1-2-4-9-17-13(16)11-6-5-7-12(15)10-11/h5-7,10H,1-4,8
InchiKey: NUEHAAPFALIYNQ-UHFFFAOYSA-N
Formula: C13H16Cl2O2
SMILES: O=C(OCCCCCCCl)c1cccc(Cl)c1
Mol. weight [g/mol]: 275.17

Physical Properties

Property code	Value	Unit	Source
gf	-96.42	kJ/mol	Joback Method
hf	-362.87	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	65.40	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.296		Crippen Method
mcvol	202.190	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	679.65	K	Joback Method
tc	890.73	K	Joback Method
tf	407.21	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.04	J/mol×K	679.65	Joback Method
cpg	557.78	J/mol×K	855.55	Joback Method
cpg	547.45	J/mol×K	820.37	Joback Method
cpg	536.34	J/mol×K	785.19	Joback Method
cpg	524.42	J/mol×K	750.01	Joback Method
cpg	511.66	J/mol×K	714.83	Joback Method
cpg	567.34	J/mol×K	890.73	Joback Method
dvisc	0.0001435	Pa×s	679.65	Joback Method

dvisc	0.0001815	Pa×s	634.24	Joback Method
dvisc	0.0002379	Pa×s	588.84	Joback Method
dvisc	0.0003264	Pa×s	543.43	Joback Method
dvisc	0.0004743	Pa×s	498.02	Joback Method
dvisc	0.0007429	Pa×s	452.62	Joback Method
dvisc	0.0012860	Pa×s	407.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357397&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