4-Chlorobenzoic acid, hexyl ester

Other names: Hexyl 4-chlorobenzoate
Inchi: InChI=1S/C13H17ClO2/c1-2-3-4-5-10-16-13(15)11-6-8-12(14)9-7-11/h6-9H,2-5,10H2,1H
InchiKey: WNIDDGDBCDWAIE-UHFFFAOYSA-N
Formula: C13H17ClO2
SMILES: CCCCCCOC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 240.73
CAS: 58435-21-5

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	-4.49		Crippen Method
logp	4.077		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1735.00		NIST Webbook
ripol	2268.00		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2248.00		NIST Webbook
ripol	2254.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2297.00		NIST Webbook
ripol	2254.00		NIST Webbook
tb	642.22	K	Joback Method
tc	849.84	K	Joback Method
tf	377.29	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.36	J/mol×K	642.22	Joback Method
cpg	485.98	J/mol×K	676.82	Joback Method
cpg	499.75	J/mol×K	711.43	Joback Method
cpg	512.68	J/mol×K	746.03	Joback Method
cpg	524.81	J/mol×K	780.63	Joback Method
cpg	536.14	J/mol×K	815.23	Joback Method
cpg	546.71	J/mol×K	849.84	Joback Method
dvisc	0.0014793	Pa×s	377.29	Joback Method
dvisc	0.0008357	Pa×s	421.45	Joback Method
dvisc	0.0005262	Pa×s	465.60	Joback Method
dvisc	0.0003589	Pa×s	509.75	Joback Method
dvisc	0.0002602	Pa×s	553.91	Joback Method
dvisc	0.0001978	Pa×s	598.07	Joback Method
dvisc	0.0001562	Pa×s	642.22	Joback Method

Sources

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=C58435215&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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