Hexan-3-yl 3-chlorobenzoate

Inchi: InChI=1S/C13H17ClO2/c1-3-6-12(4-2)16-13(15)10-7-5-8-11(14)9-10/h5,7-9,12H,3-4,6H2
InchiKey: AOCUMMOCVLVVHT-UHFFFAOYSA-N
Formula: C13H17ClO2
SMILES: CCCC(CC)OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 240.73

Physical Properties

Property code	Value	Unit	Source
gf	-86.93	kJ/mol	Joback Method
hf	-352.41	kJ/mol	Joback Method
hfus	26.54	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.075		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	641.78	K	Joback Method
tc	853.39	K	Joback Method
tf	362.29	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.84	J/mol×K	641.78	Joback Method
cpg	537.80	J/mol×K	818.12	Joback Method
cpg	526.31	J/mol×K	782.85	Joback Method
cpg	513.99	J/mol×K	747.58	Joback Method
cpg	500.82	J/mol×K	712.32	Joback Method
cpg	486.78	J/mol×K	677.05	Joback Method
cpg	548.48	J/mol×K	853.39	Joback Method
dvisc	0.0001452	Pa×s	641.78	Joback Method

dvisc	0.0001874	Pa×s	595.20	Joback Method
dvisc	0.0002527	Pa×s	548.62	Joback Method
dvisc	0.0003601	Pa×s	502.03	Joback Method
dvisc	0.0005517	Pa×s	455.45	Joback Method
dvisc	0.0009315	Pa×s	408.87	Joback Method
dvisc	0.0017997	Pa×s	362.29	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373573&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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