10-Chlorodecyl 3-chlorobenzoate

Inchi: InChI=1S/C17H24Cl2O2/c18-12-7-5-3-1-2-4-6-8-13-21-17(20)15-10-9-11-16(19)14-15/h9
InchiKey: OFBFSHCSGLYCEN-UHFFFAOYSA-N
Formula: C17H24Cl2O2
SMILES: O=C(OCCCCCCCCCCCl)c1cccc(Cl)c1
Mol. weight [g/mol]: 331.28

Physical Properties

Property code	Value	Unit	Source
gf	-62.74	kJ/mol	Joback Method
hf	-445.43	kJ/mol	Joback Method
hfus	44.62	kJ/mol	Joback Method
hvap	74.30	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.856		Crippen Method
mcvol	258.550	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2500.00		NIST Webbook
tb	771.17	K	Joback Method
tc	973.24	K	Joback Method
tf	452.29	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.52	J/mol×K	771.17	Joback Method
cpg	728.71	J/mol×K	804.85	Joback Method
cpg	742.94	J/mol×K	838.53	Joback Method
cpg	756.25	J/mol×K	872.20	Joback Method
cpg	768.66	J/mol×K	905.88	Joback Method
cpg	780.20	J/mol×K	939.56	Joback Method
cpg	790.92	J/mol×K	973.24	Joback Method
dvisc	0.0009311	Pa×s	452.29	Joback Method
dvisc	0.0005082	Pa×s	505.44	Joback Method

dvisc	0.0003113	Pa×s	558.58	Joback Method
dvisc	0.0002076	Pa×s	611.73	Joback Method
dvisc	0.0001477	Pa×s	664.88	Joback Method
dvisc	0.0001105	Pa×s	718.02	Joback Method
dvisc	0.0000861	Pa×s	771.17	Joback Method

Sources

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=U373564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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