(E)-Dodec-2-enyl 3-chlorobenzoate

Inchi: InChI=1S/C19H27ClO2/c1-2-3-4-5-6-7-8-9-10-11-15-22-19(21)17-13-12-14-18(20)16-17/
InchiKey: FNGCCVRQRRRMQZ-ZHACJKMWSA-N
Formula: C19H27ClO2
SMILES: CCCCCCCCCC=CCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 322.87

Physical Properties

Property code	Value	Unit	Source
gf	46.25	kJ/mol	Joback Method
hf	-353.75	kJ/mol	Joback Method
hfus	45.80	kJ/mol	Joback Method
hvap	74.33	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.194		Crippen Method
mcvol	270.190	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2388.00		NIST Webbook
tb	783.66	K	Joback Method
tc	985.06	K	Joback Method
tf	439.83	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.81	J/mol×K	783.66	Joback Method
cpg	846.24	J/mol×K	951.49	Joback Method
cpg	833.55	J/mol×K	917.92	Joback Method
cpg	820.00	J/mol×K	884.36	Joback Method
cpg	805.56	J/mol×K	850.79	Joback Method
cpg	790.18	J/mol×K	817.23	Joback Method
cpg	858.15	J/mol×K	985.06	Joback Method
dvisc	0.0000652	Pa×s	783.66	Joback Method
dvisc	0.0000847	Pa×s	726.36	Joback Method

dvisc	0.0001150	Pa×s	669.05	Joback Method
dvisc	0.0001655	Pa×s	611.75	Joback Method
dvisc	0.0002566	Pa×s	554.44	Joback Method
dvisc	0.0004404	Pa×s	497.14	Joback Method
dvisc	0.0008699	Pa×s	439.83	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=U373542&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume