

(Z)-Dec-4-enyl 3-chlorobenzoate

Inchi:	InChI=1S/C17H23ClO2/c1-2-3-4-5-6-7-8-9-13-20-17(19)15-11-10-12-16(18)14-15/h6-7,1
InchiKey:	VOLMYSSMSCCCBL-SREVYHEPSA-N
Formula:	C17H23ClO2
SMILES:	CCCCC=CCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	294.82

Physical Properties

Property code	Value	Unit	Source
gf	29.41	kJ/mol	Joback Method
hf	-312.47	kJ/mol	Joback Method
hfus	40.62	kJ/mol	Joback Method
hvap	69.87	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.413		Crippen Method
mcvol	242.010	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	737.90	K	Joback Method
tc	942.28	K	Joback Method
tf	417.29	K	Joback Method
vc	0.932	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.12	J/molxK	737.90	Joback Method
cpg	730.89	J/molxK	908.22	Joback Method
cpg	718.68	J/molxK	874.16	Joback Method
cpg	705.64	J/molxK	840.09	Joback Method
cpg	691.73	J/molxK	806.03	Joback Method
cpg	676.90	J/molxK	771.96	Joback Method
cpg	742.32	J/molxK	942.28	Joback Method
dvisc	0.0000843	Paxs	737.90	Joback Method

dvisc	0.0001088	Paxs	684.46	Joback Method
dvisc	0.0001466	Paxs	631.03	Joback Method
dvisc	0.0002087	Paxs	577.60	Joback Method
dvisc	0.0003193	Paxs	524.16	Joback Method
dvisc	0.0005380	Paxs	470.73	Joback Method
dvisc	0.0010361	Paxs	417.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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