

(Z)-Non-3-enyl 3-chlorobenzoate

Inchi:	InChI=1S/C16H21ClO2/c1-2-3-4-5-6-7-8-12-19-16(18)14-10-9-11-15(17)13-14/h6-7,9-11
InchiKey:	SHIPTPLHQXDWPB-SREVYHEPSA-N
Formula:	C16H21ClO2
SMILES:	CCCCC=CCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	280.79

Physical Properties

Property code	Value	Unit	Source
gf	20.99	kJ/mol	Joback Method
hf	-291.83	kJ/mol	Joback Method
hfus	38.03	kJ/mol	Joback Method
hvap	67.65	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.023		Crippen Method
mvol	227.920	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	2054.00		NIST Webbook
tb	715.02	K	Joback Method
tc	921.66	K	Joback Method
tf	406.02	K	Joback Method
vc	0.876	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.40	J/molxK	715.02	Joback Method
cpg	621.84	J/molxK	749.46	Joback Method
cpg	636.34	J/molxK	783.90	Joback Method
cpg	649.93	J/molxK	818.34	Joback Method
cpg	662.67	J/molxK	852.78	Joback Method
cpg	674.59	J/molxK	887.22	Joback Method
cpg	685.73	J/molxK	921.66	Joback Method
dvisc	0.0011208	Paxs	406.02	Joback Method
dvisc	0.0005899	Paxs	457.52	Joback Method

dvisc	0.0003536	Paxs	509.02	Joback Method
dvisc	0.0002328	Paxs	560.52	Joback Method
dvisc	0.0001645	Paxs	612.02	Joback Method
dvisc	0.0001226	Paxs	663.52	Joback Method
dvisc	0.0000954	Paxs	715.02	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373553&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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