3-Chlorobenzoic acid, neopentyl ester

Other names: 3-Chlorobenzoic acid, neopentyl ester
Inchi: InChI=1S/C12H15ClO2/c1-12(2,3)8-15-11(14)9-5-4-6-10(13)7-9/h4-7H,8H2,1-3H3
InchiKey: HKBVGVISHWBWGQ-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: CC(C)(C)COC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 226.70

Physical Properties

Property code	Value	Unit	Source
hf	-421.84	kJ/mol	Cheméo Relay (1.0)
hfus	20.06	kJ/mol	Joback Method
hvap	68.79	kJ/mol	Cheméo Relay (1.0)
ie	9.30	eV	Cheméo Relay (1.0)
log10ws	-4.72		Cheméo Relay (1.0)
logp	3.543		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1537.00		NIST Webbook
tb	548.54	K	Cheméo Relay (1.0)
tc	749.42	K	Cheméo Relay (1.0)
tf	344.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.66	J/mol×K	616.11	Joback Method
cpg	439.36	J/mol×K	653.34	Joback Method
cpg	453.06	J/mol×K	690.57	Joback Method
cpg	465.80	J/mol×K	727.79	Joback Method
cpg	477.62	J/mol×K	765.02	Joback Method
cpg	488.58	J/mol×K	802.25	Joback Method
cpg	498.71	J/mol×K	839.48	Joback Method
dvisc	0.0016900	Pa×s	368.44	Joback Method

dvisc	0.0009254	Pa×s	409.72	Joback Method
dvisc	0.0005657	Pa×s	451.00	Joback Method
dvisc	0.0003756	Pa×s	492.27	Joback Method
dvisc	0.0002657	Pa×s	533.55	Joback Method
dvisc	0.0001975	Pa×s	574.83	Joback Method
dvisc	0.0001528	Pa×s	616.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C343775315&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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