Neopentyl 3-chlorobenzoate

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
CAS: 343775-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-90.07	kJ/mol	Joback Method
hf	-335.24	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	57.49	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
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	616.11	K	Joback Method
tc	839.48	K	Joback Method
tf	368.44	K	Joback Method
vc	0.661	m3/kmol	Joback Method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C343775315&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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