

Carbonic acid, neopentyl 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C12H14Cl2O3/c1-12(2,3)7-16-11(15)17-8-4-5-9(13)10(14)6-8/h4-6H,7H2,1-3H
InchiKey:	HJNFYEFJFLFVLX-UHFFFAOYSA-N
Formula:	C12H14Cl2O3
SMILES:	CC(C)(C)COC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	277.14

Physical Properties

Property code	Value	Unit	Source
gf	-216.63	kJ/mol	Joback Method
hf	-494.67	kJ/mol	Joback Method
hfus	25.05	kJ/mol	Joback Method
hvap	64.95	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.555		Crippen Method
mcvol	193.970	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinqol	1777.00		NIST Webbook
tb	680.94	K	Joback Method
tc	905.46	K	Joback Method
tf	433.11	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.15	J/molxK	680.94	Joback Method
cpg	487.23	J/molxK	718.36	Joback Method
cpg	499.39	J/molxK	755.78	Joback Method
cpg	510.65	J/molxK	793.20	Joback Method
cpg	521.04	J/molxK	830.62	Joback Method
cpg	530.58	J/molxK	868.04	Joback Method
cpg	539.30	J/molxK	905.46	Joback Method
dvisc	0.0008237	Paxs	433.11	Joback Method
dvisc	0.0005039	Paxs	474.42	Joback Method

dvisc	0.0003335	Paxs	515.72	Joback Method
dvisc	0.0002347	Paxs	557.02	Joback Method
dvisc	0.0001733	Paxs	598.33	Joback Method
dvisc	0.0001331	Paxs	639.63	Joback Method
dvisc	0.0001056	Paxs	680.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357864&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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