

Carbonic acid, propyl 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C10H10Cl2O3/c1-2-5-14-10(13)15-7-3-4-8(11)9(12)6-7/h3-4,6H,2,5H2,1H3
InchiKey:	KPKUZTHEGNXGQU-UHFFFAOYSA-N
Formula:	C10H10Cl2O3
SMILES:	CCCOC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	249.09

Physical Properties

Property code	Value	Unit	Source
gf	-236.31	kJ/mol	Joback Method
hf	-444.64	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	61.79	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.919		Crippen Method
mcvol	165.790	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1689.00		NIST Webbook
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tb	638.41	K	Joback Method
tc	858.50	K	Joback Method
tf	408.15	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.26	J/molxK	638.41	Joback Method
cpg	383.53	J/molxK	675.09	Joback Method
cpg	394.13	J/molxK	711.77	Joback Method
cpg	404.04	J/molxK	748.45	Joback Method
cpg	413.26	J/molxK	785.14	Joback Method
cpg	421.79	J/molxK	821.82	Joback Method
cpg	429.62	J/molxK	858.50	Joback Method
dvisc	0.0009285	Paxs	408.15	Joback Method

dvisc	0.0006073	Paxs	446.53	Joback Method
dvisc	0.0004249	Paxs	484.90	Joback Method
dvisc	0.0003132	Paxs	523.28	Joback Method
dvisc	0.0002407	Paxs	561.66	Joback Method
dvisc	0.0001913	Paxs	600.03	Joback Method
dvisc	0.0001564	Paxs	638.41	Joback Method

Sources

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=U357822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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