

Carbonic acid, ethyl 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C9H8Cl2O3/c1-2-13-9(12)14-6-3-4-7(10)8(11)5-6/h3-5H,2H2,1H3
InchiKey:	IHBKIQNCLUJXCK-UHFFFAOYSA-N
Formula:	C9H8Cl2O3
SMILES:	CCOC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	235.06

Physical Properties

Property code	Value	Unit	Source
gf	-244.73	kJ/mol	Joback Method
hf	-424.00	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	59.56	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.529		Crippen Method
mcvol	151.700	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1578.00		NIST Webbook
rinpol	1578.00		NIST Webbook
tb	615.53	K	Joback Method
tc	839.68	K	Joback Method
tf	396.88	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.15	J/mol×K	615.53	Joback Method
cpg	370.91	J/mol×K	802.32	Joback Method
cpg	363.02	J/mol×K	764.96	Joback Method
cpg	354.49	J/mol×K	727.60	Joback Method
cpg	345.33	J/mol×K	690.25	Joback Method
cpg	335.55	J/mol×K	652.89	Joback Method
cpg	378.14	J/mol×K	839.68	Joback Method
dvisc	0.0001737	Pa×s	615.53	Joback Method

dvisc	0.0002115	Pa×s	579.09	Joback Method
dvisc	0.0002642	Pa×s	542.65	Joback Method
dvisc	0.0003410	Pa×s	506.20	Joback Method
dvisc	0.0004578	Pa×s	469.76	Joback Method
dvisc	0.0006457	Pa×s	433.32	Joback Method
dvisc	0.0009703	Pa×s	396.88	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=U357922&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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