

Carbonic acid, allyl 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C10H8Cl2O3/c1-2-6-14-10(13)15-8-5-3-4-7(11)9(8)12/h2-5H,1,6H2
InchiKey:	HAGVVWNFFJJGGZ-UHFFFAOYSA-N
Formula:	C10H8Cl2O3
SMILES:	C=CCOC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	247.07

Physical Properties

Property code	Value	Unit	Source
gf	-148.47	kJ/mol	Joback Method
hf	-319.21	kJ/mol	Joback Method
hfus	26.01	kJ/mol	Joback Method
hvap	61.12	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.695		Crippen Method
mcvol	161.490	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpola	1660.00		NIST Webbook
tb	635.09	K	Joback Method
tc	859.63	K	Joback Method
tf	406.39	K	Joback Method
vc	0.609	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.72	J/molxK	635.09	Joback Method
cpg	361.24	J/molxK	672.51	Joback Method
cpg	371.09	J/molxK	709.94	Joback Method
cpg	380.27	J/molxK	747.36	Joback Method
cpg	388.78	J/molxK	784.78	Joback Method
cpg	396.62	J/molxK	822.20	Joback Method
cpg	403.78	J/molxK	859.63	Joback Method
dvisc	0.0009192	Paxs	406.39	Joback Method
dvisc	0.0006090	Paxs	444.51	Joback Method

dvisc	0.0004306	Paxs	482.62	Joback Method
dvisc	0.0003203	Paxs	520.74	Joback Method
dvisc	0.0002481	Paxs	558.86	Joback Method
dvisc	0.0001985	Paxs	596.97	Joback Method
dvisc	0.0001632	Paxs	635.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357381&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

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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