

Carbonic acid, allyl 4-chlorophenyl ester

Inchi: InChI=1S/C10H9ClO3/c1-2-7-13-10(12)14-9-5-3-8(11)4-6-9/h2-6H,1,7H2
InchiKey: VQLKYCRDMAFZRI-UHFFFAOYSA-N
Formula: C10H9ClO3
SMILES: C=CCOC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 212.63

Physical Properties

Property code	Value	Unit	Source
gf	-126.91	kJ/mol	Joback Method
hf	-292.00	kJ/mol	Joback Method
hfus	22.20	kJ/mol	Joback Method
hvap	56.07	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.041		Crippen Method
mcvol	149.250	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	1500.00		NIST Webbook
tb	592.68	K	Joback Method
tc	812.73	K	Joback Method
tf	363.95	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.95	J/mol×K	592.68	Joback Method
cpg	340.51	J/mol×K	629.35	Joback Method
cpg	351.39	J/mol×K	666.03	Joback Method
cpg	361.57	J/mol×K	702.70	Joback Method
cpg	371.08	J/mol×K	739.38	Joback Method
cpg	379.91	J/mol×K	776.05	Joback Method
cpg	388.07	J/mol×K	812.73	Joback Method
dvisc	0.0012159	Pa×s	363.95	Joback Method
dvisc	0.0007547	Pa×s	402.07	Joback Method

dvisc	0.0005088	Pa×s	440.19	Joback Method
dvisc	0.0003652	Pa×s	478.32	Joback Method
dvisc	0.0002753	Pa×s	516.44	Joback Method
dvisc	0.0002158	Pa×s	554.56	Joback Method
dvisc	0.0001745	Pa×s	592.68	Joback Method

Sources

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=U357809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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