

Carbonic acid, allyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C11H12O4/c1-3-8-14-11(12)15-10-6-4-9(13-2)5-7-10/h3-7H,1,8H2,2H3
InchiKey:	XGLNRGJVKCXSPM-UHFFFAOYSA-N
Formula:	C11H12O4
SMILES:	C=CCOC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	208.21

Physical Properties

Property code	Value	Unit	Source
gf	-211.56	kJ/mol	Joback Method
hf	-429.12	kJ/mol	Joback Method
hfus	21.78	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.397		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
tb	600.55	K	Joback Method
tc	810.56	K	Joback Method
tf	367.53	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.75	J/mol×K	600.55	Joback Method
cpg	387.78	J/mol×K	635.55	Joback Method
cpg	400.13	J/mol×K	670.55	Joback Method
cpg	411.79	J/mol×K	705.56	Joback Method
cpg	422.75	J/mol×K	740.56	Joback Method
cpg	433.00	J/mol×K	775.56	Joback Method
cpg	442.53	J/mol×K	810.56	Joback Method
dvisc	0.0009577	Pa×s	367.53	Joback Method

dvisc	0.0005880	Pa×s	406.37	Joback Method
dvisc	0.0003931	Pa×s	445.20	Joback Method
dvisc	0.0002804	Pa×s	484.04	Joback Method
dvisc	0.0002102	Pa×s	522.88	Joback Method
dvisc	0.0001641	Pa×s	561.71	Joback Method
dvisc	0.0001322	Pa×s	600.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357810&Units=SI
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

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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