

Carbonic acid, allyl 3-methylphenyl ester

Inchi:	InChI=1S/C11H12O3/c1-3-7-13-11(12)14-10-6-4-5-9(2)8-10/h3-6,8H,1,7H2,2H3
InchiKey:	CLOWDQOEQBVSPC-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	C=CCOC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	192.21

Physical Properties

Property code	Value	Unit	Source
gf	-106.56	kJ/mol	Joback Method
hf	-296.90	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.696		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinsol	1432.00		NIST Webbook
tb	578.13	K	Joback Method
tc	790.48	K	Joback Method
tf	345.30	K	Joback Method
vc	0.567	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.57	J/molxK	578.13	Joback Method
cpg	409.62	J/molxK	755.09	Joback Method
cpg	399.22	J/molxK	719.70	Joback Method
cpg	388.12	J/molxK	684.30	Joback Method
cpg	376.32	J/molxK	648.91	Joback Method
cpg	363.80	J/molxK	613.52	Joback Method
cpg	419.32	J/molxK	790.48	Joback Method
dvisc	0.0001641	Paxs	578.13	Joback Method
dvisc	0.0002041	Paxs	539.33	Joback Method

dvisc	0.0002626	Paxs	500.52	Joback Method
dvisc	0.0003525	Paxs	461.72	Joback Method
dvisc	0.0004995	Paxs	422.91	Joback Method
dvisc	0.0007593	Paxs	384.11	Joback Method
dvisc	0.0012684	Paxs	345.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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