Carbonic acid, allyl 4-benzyloxyphenyl ester

Inchi: InChI=1S/C17H16O4/c1-2-12-19-17(18)21-16-10-8-15(9-11-16)20-13-14-6-4-3-5-7-14/h2
InchiKey: GKDJASGAZGOOQZ-UHFFFAOYSA-N
Formula: C17H16O4
SMILES: C=CCOC(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 284.31

Physical Properties

Property code	Value	Unit	Source
gf	-48.63	kJ/mol	Joback Method
hf	-316.43	kJ/mol	Joback Method
hfus	31.36	kJ/mol	Joback Method
hvap	71.96	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.967		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	2307.00		NIST Webbook
tb	764.51	K	Joback Method
tc	992.34	K	Joback Method
tf	461.57	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.21	J/mol×K	764.51	Joback Method
cpg	614.91	J/mol×K	802.48	Joback Method
cpg	628.40	J/mol×K	840.45	Joback Method
cpg	640.70	J/mol×K	878.43	Joback Method
cpg	651.83	J/mol×K	916.40	Joback Method
cpg	661.80	J/mol×K	954.37	Joback Method
cpg	670.64	J/mol×K	992.34	Joback Method
dvisc	0.0005752	Pa×s	461.57	Joback Method
dvisc	0.0003390	Pa×s	512.06	Joback Method

dvisc	0.0002197	Pa×s	562.55	Joback Method
dvisc	0.0001530	Pa×s	613.04	Joback Method
dvisc	0.0001125	Pa×s	663.53	Joback Method
dvisc	0.0000864	Pa×s	714.02	Joback Method
dvisc	0.0000688	Pa×s	764.51	Joback Method

Sources

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=U357813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/58-001-6/Carbonic-acid-allyl-4-benzyloxyphenyl-ester.pdf
Generated by Cheméo on 2024-10-12 08:55:45.555614317 +0000 UTC m=+3304208.192583565.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.