Carbonic acid, allyl 4-isopropylphenyl ester

Inchi: InChI=1S/C13H16O3/c1-4-9-15-13(14)16-12-7-5-11(6-8-12)10(2)3/h4-8,10H,1,9H2,2-3H
InchiKey: HGLOCQRSJASENM-UHFFFAOYSA-N
Formula: C13H16O3
SMILES: C=CCOC(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]: 220.26

Physical Properties

Property code	Value	Unit	Source
gf	-92.16	kJ/mol	Joback Method
hf	-343.46	kJ/mol	Joback Method
hfus	22.25	kJ/mol	Joback Method
hvap	57.98	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.511		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1591.00		NIST Webbook
tb	623.45	K	Joback Method
tc	833.19	K	Joback Method
tf	352.84	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.15	J/mol×K	623.45	Joback Method
cpg	463.15	J/mol×K	658.41	Joback Method
cpg	477.30	J/mol×K	693.36	Joback Method
cpg	490.60	J/mol×K	728.32	Joback Method
cpg	503.08	J/mol×K	763.28	Joback Method
cpg	514.73	J/mol×K	798.23	Joback Method
cpg	525.57	J/mol×K	833.19	Joback Method
dvisc	0.0014541	Pa×s	352.84	Joback Method
dvisc	0.0007699	Pa×s	397.94	Joback Method

dvisc	0.0004640	Pa×s	443.04	Joback Method
dvisc	0.0003070	Pa×s	488.15	Joback Method
dvisc	0.0002179	Pa×s	533.25	Joback Method
dvisc	0.0001631	Pa×s	578.35	Joback Method
dvisc	0.0001273	Pa×s	623.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357380&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