Carbonic acid, allyl cyclohexylmethyl ester

Inchi: InChI=1S/C11H18O3/c1-2-8-13-11(12)14-9-10-6-4-3-5-7-10/h2,10H,1,3-9H2
InchiKey: XJXMUGUGYJEXGN-UHFFFAOYSA-N
Formula: C11H18O3
SMILES: C=CCOC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 198.26

Physical Properties

Property code	Value	Unit	Source
gf	-184.89	kJ/mol	Joback Method
hf	-467.64	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	51.41	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.906		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1421.00		NIST Webbook
rinpol	1421.00		NIST Webbook
tb	566.02	K	Joback Method
tc	770.50	K	Joback Method
tf	313.74	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.52	J/mol×K	566.02	Joback Method
cpg	429.06	J/mol×K	600.10	Joback Method
cpg	445.69	J/mol×K	634.18	Joback Method
cpg	461.44	J/mol×K	668.26	Joback Method
cpg	476.30	J/mol×K	702.34	Joback Method
cpg	490.28	J/mol×K	736.42	Joback Method
cpg	503.38	J/mol×K	770.50	Joback Method
dvisc	0.0027116	Pa×s	313.74	Joback Method

dvisc	0.0013277	Pa×s	355.79	Joback Method
dvisc	0.0007561	Pa×s	397.83	Joback Method
dvisc	0.0004794	Pa×s	439.88	Joback Method
dvisc	0.0003292	Pa×s	481.93	Joback Method
dvisc	0.0002401	Pa×s	523.97	Joback Method
dvisc	0.0001835	Pa×s	566.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357807&Units=SI

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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