Cyclohexanepropanoic acid, 2-propenyl ester

Other names:	Cyclohexanepropionic acid, allyl ester
	Allyl cyclohexanepropionate
	Allyl cyclohexylpropionate
	3-Allylcyclohexyl propionate
	Allyl hexahydrophenylpropionate
	Cyclohexanol, 3-allyl-, propionate
	Ananolide
	Allyl-3-cyclohexyl propionate
	Propanoic acid, 3-cyclohexyl, 2-propenyl ester
	allyl cyclohexylpropanoate
Inchi:	InChI=1S/C12H20O2/c1-2-10-14-12(13)9-8-11-6-4-3-5-7-11/h2,11H,1,3-10H2
InchiKey:	TWXUTZNBHUWMKJ-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	C=CCOC(=O)CCC1CCCCC1
Mol. weight [g/mol]:	196.29
CAS:	2705-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-71.47	kJ/mol	Joback Method
hf	-356.06	kJ/mol	Joback Method
hfus	20.18	kJ/mol	Joback Method
hvap	51.22	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.076		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1406.70		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1407.00		NIST Webbook
ripol	1826.00		NIST Webbook
ripol	1778.00		NIST Webbook
ripol	1800.00		NIST Webbook

ripol	1800.00		NIST Webbook
tb	566.48	K	Joback Method
tc	769.87	K	Joback Method
tf	302.78	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.02	J/mol×K	566.48	Joback Method
cpg	452.58	J/mol×K	600.38	Joback Method
cpg	470.15	J/mol×K	634.28	Joback Method
cpg	486.75	J/mol×K	668.18	Joback Method
cpg	502.40	J/mol×K	702.08	Joback Method
cpg	517.12	J/mol×K	735.97	Joback Method
cpg	530.94	J/mol×K	769.87	Joback Method
dvisc	0.0036730	Pa×s	302.78	Joback Method
dvisc	0.0016805	Pa×s	346.73	Joback Method
dvisc	0.0009168	Pa×s	390.68	Joback Method
dvisc	0.0005653	Pa×s	434.63	Joback Method
dvisc	0.0003810	Pa×s	478.58	Joback Method
dvisc	0.0002744	Pa×s	522.53	Joback Method
dvisc	0.0002079	Pa×s	566.48	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=C2705875&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume