3-Cyclopentylpropionic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C11H17ClO2/c12-8-3-9-14-11(13)7-6-10-4-1-2-5-10/h3,8,10H,1-2,4-7,9H2/b8-3

InchiKey: QXWNSXGSUGCIHO-FPYGCLRLSA-N

Formula: C11H17ClO2

SMILES: O=C(CCC1CCCC1)OCC=CCl

Mol. weight [g/mol]: 216.70

Physical Properties

Property code	Value	Unit	Source
gf	-87.34	kJ/mol	Joback Method
hf	-353.21	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	53.84	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.252		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1555.10		NIST Webbook
rinpol	1555.10		NIST Webbook
tb	584.24	K	Joback Method
tc	792.73	K	Joback Method
tf	321.63	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.39	J/mol×K	584.24	Joback Method
cpg	431.62	J/mol×K	618.99	Joback Method
cpg	446.89	J/mol×K	653.74	Joback Method
cpg	461.25	J/mol×K	688.48	Joback Method
cpg	474.73	J/mol×K	723.23	Joback Method
cpg	487.37	J/mol×K	757.98	Joback Method
cpg	499.21	J/mol×K	792.73	Joback Method
dvisc	0.0027862	Pa×s	321.63	Joback Method

dvisc	0.0014396	Pa×s	365.40	Joback Method
dvisc	0.0008567	Pa×s	409.17	Joback Method
dvisc	0.0005636	Pa×s	452.94	Joback Method
dvisc	0.0003992	Pa×s	496.70	Joback Method
dvisc	0.0002990	Pa×s	540.47	Joback Method
dvisc	0.0002338	Pa×s	584.24	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=U292472&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