

Cyclopropanecarboxylic acid, oct-3-en-2-yl ester

Inchi:	InChI=1S/C12H20O2/c1-3-4-5-6-7-10(2)14-12(13)11-8-9-11/h6-7,10-11H,3-5,8-9H2,1-2H
InchiKey:	WTBNOXVDMAKPIY-VOTSOKGWSA-N
Formula:	C12H20O2
SMILES:	CCCCC=CC(C)OC(=O)C1CC1
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
gf	-45.23	kJ/mol	Joback Method
hf	-351.07	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.075		Crippen Method
mvol	172.220	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1346.00		NIST Webbook
tb	560.71	K	Joback Method
tc	752.87	K	Joback Method
tf	295.02	K	Joback Method
vc	0.662	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.25	J/molxK	560.71	Joback Method
cpg	506.04	J/molxK	720.84	Joback Method
cpg	492.86	J/molxK	688.81	Joback Method
cpg	478.93	J/molxK	656.79	Joback Method
cpg	464.22	J/molxK	624.76	Joback Method
cpg	448.67	J/molxK	592.74	Joback Method
cpg	518.51	J/molxK	752.87	Joback Method
dvisc	0.0003339	Paxs	560.71	Joback Method
dvisc	0.0004078	Paxs	516.43	Joback Method

dvisc	0.0005170	Paxs	472.15	Joback Method
dvisc	0.0006885	Paxs	427.87	Joback Method
dvisc	0.0009795	Paxs	383.58	Joback Method
dvisc	0.0015280	Paxs	339.30	Joback Method
dvisc	0.0027239	Paxs	295.02	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=U299377&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

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