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

Inchi: InChI=1S/C13H22O2/c1-3-4-5-6-8-11(2)15-13(14)12-9-7-10-12/h6,8,11-12H,3-5,7,9-10H

InchiKey: XJSRLKXXHRKVIC-SOFGYWHQSA-N

Formula: C13H22O2

SMILES: CCCCC=CC(C)OC(=O)C1CCC1

Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-48.91	kJ/mol	Joback Method
hf	-377.87	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.465		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1423.00		NIST Webbook
tb	587.86	K	Joback Method
tc	783.78	K	Joback Method
tf	302.77	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.98	J/mol×K	587.86	Joback Method
cpg	501.78	J/mol×K	620.51	Joback Method
cpg	518.63	J/mol×K	653.17	Joback Method
cpg	534.56	J/mol×K	685.82	Joback Method
cpg	549.61	J/mol×K	718.47	Joback Method
cpg	563.82	J/mol×K	751.12	Joback Method
cpg	577.24	J/mol×K	783.78	Joback Method
dvisc	0.0032396	Pa×s	302.77	Joback Method
dvisc	0.0015717	Pa×s	350.28	Joback Method

dvisc	0.0009063	Pa×s	397.80	Joback Method
dvisc	0.0005878	Pa×s	445.31	Joback Method
dvisc	0.0004144	Pa×s	492.83	Joback Method
dvisc	0.0003107	Pa×s	540.35	Joback Method
dvisc	0.0002440	Pa×s	587.86	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=U299132&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