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

Inchi: InChI=1S/C16H28O2/c1-3-4-5-6-9-14(2)18-16(17)13-12-15-10-7-8-11-15/h6,9,14-15H,3-

InchiKey: RVRMKAKPHWJDJO-RMKNXTFCSA-N

Formula: C16H28O2

SMILES: CCCCC=CC(C)OC(=O)CCC1CCCC1

Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	-35.75	kJ/mol	Joback Method
hf	-445.95	kJ/mol	Joback Method
hfus	30.60	kJ/mol	Joback Method
hvap	60.19	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.635		Crippen Method
mcvol	228.580	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	1742.50		NIST Webbook
rinpol	1742.50		NIST Webbook
tb	660.77	K	Joback Method
tc	855.42	K	Joback Method
tf	333.06	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.22	J/mol×K	660.77	Joback Method
cpg	666.91	J/mol×K	693.21	Joback Method
cpg	685.51	J/mol×K	725.65	Joback Method
cpg	703.09	J/mol×K	758.09	Joback Method
cpg	719.66	J/mol×K	790.53	Joback Method
cpg	735.28	J/mol×K	822.98	Joback Method
cpg	750.00	J/mol×K	855.42	Joback Method
dvisc	0.0032081	Pa×s	333.06	Joback Method

dvisc	0.0013140	Pa×s	387.68	Joback Method
dvisc	0.0006709	Pa×s	442.30	Joback Method
dvisc	0.0003971	Pa×s	496.91	Joback Method
dvisc	0.0002608	Pa×s	551.53	Joback Method
dvisc	0.0001847	Pa×s	606.15	Joback Method
dvisc	0.0001385	Pa×s	660.77	Joback Method

Sources

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=U292468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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