

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

Inchi:	InChI=1S/C18H24O2/c1-3-4-5-7-10-14(2)20-18(19)17-13-16(17)15-11-8-6-9-12-15/h6-12
InchiKey:	YMMIEKBQBRAIEL-JXMROGBWSA-N
Formula:	C18H24O2
SMILES:	CCCCC=CC(C)OC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
gf	109.99	kJ/mol	Joback Method
hf	-258.72	kJ/mol	Joback Method
hfus	35.09	kJ/mol	Joback Method
hvap	66.27	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.468		Crippen Method
mcvol	233.000	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	720.00	K	Joback Method
tc	932.25	K	Joback Method
tf	384.82	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.77	J/molxK	720.00	Joback Method
cpg	694.16	J/molxK	755.37	Joback Method
cpg	711.38	J/molxK	790.75	Joback Method
cpg	727.50	J/molxK	826.12	Joback Method
cpg	742.60	J/molxK	861.50	Joback Method
cpg	756.75	J/molxK	896.87	Joback Method
cpg	770.03	J/molxK	932.25	Joback Method
dvisc	0.0019315	Paxs	384.82	Joback Method

dvisc	0.0011188	Paxs	440.68	Joback Method
dvisc	0.0007328	Paxs	496.55	Joback Method
dvisc	0.0005229	Paxs	552.41	Joback Method
dvisc	0.0003969	Paxs	608.27	Joback Method
dvisc	0.0003156	Paxs	664.14	Joback Method
dvisc	0.0002601	Paxs	720.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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