Cyclopropanecarboxylic acid, trans-2-phenyl-, octadecyl ester

Inchi: InChI=1S/C28H46O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-30-28(29)27-24-26
InchiKey: IEFIGJUOZNQAAS-UHFFFAOYSA-N
Formula: C28H46O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]: 414.66

Physical Properties

Property code	Value	Unit	Source
gf	116.41	kJ/mol	Joback Method
hf	-577.06	kJ/mol	Joback Method
hfus	64.31	kJ/mol	Joback Method
hvap	88.96	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.595		Crippen Method
mcvol	378.200	ml/mol	McGowan Method
pc	849.00	kPa	Joback Method
rinpol	3184.00		NIST Webbook
rinpol	3184.00		NIST Webbook
tb	945.08	K	Joback Method
tc	1157.05	K	Joback Method
tf	517.60	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.43	J/mol×K	945.08	Joback Method
cpg	1328.28	J/mol×K	980.41	Joback Method
cpg	1347.82	J/mol×K	1015.74	Joback Method
cpg	1366.14	J/mol×K	1051.07	Joback Method
cpg	1383.36	J/mol×K	1086.40	Joback Method
cpg	1399.55	J/mol×K	1121.72	Joback Method
cpg	1414.81	J/mol×K	1157.05	Joback Method
dvisc	0.0009956	Pa×s	517.60	Joback Method

dvisc	0.0005441	Pa×s	588.85	Joback Method
dvisc	0.0003387	Pa×s	660.09	Joback Method
dvisc	0.0002313	Pa×s	731.34	Joback Method
dvisc	0.0001690	Pa×s	802.59	Joback Method
dvisc	0.0001300	Pa×s	873.83	Joback Method
dvisc	0.0001040	Pa×s	945.08	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=U406009&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