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

Inchi: InChI=1S/C27H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-29-27(28)26-23-25(26

InchiKey: LUOVOWNFFFKCNB-UHFFFAOYSA-N

Formula: C27H44O2

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 400.64

Physical Properties

Property code	Value	Unit	Source
gf	107.99	kJ/mol	Joback Method
hf	-556.42	kJ/mol	Joback Method
hfus	61.72	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.205		Crippen Method
mcvol	364.110	ml/mol	McGowan Method
pc	898.56	kPa	Joback Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
tb	922.20	K	Joback Method
tc	1129.67	K	Joback Method
tf	506.33	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.43	J/mol×K	922.20	Joback Method
cpg	1263.88	J/mol×K	956.78	Joback Method
cpg	1283.07	J/mol×K	991.36	Joback Method
cpg	1301.08	J/mol×K	1025.94	Joback Method
cpg	1318.00	J/mol×K	1060.51	Joback Method
cpg	1333.92	J/mol×K	1095.09	Joback Method
cpg	1348.92	J/mol×K	1129.67	Joback Method
dvisc	0.0010892	Pa×s	506.33	Joback Method

dvisc	0.0006023	Pa×s	575.64	Joback Method
dvisc	0.0003783	Pa×s	644.95	Joback Method
dvisc	0.0002601	Pa×s	714.26	Joback Method
dvisc	0.0001910	Pa×s	783.58	Joback Method
dvisc	0.0001476	Pa×s	852.89	Joback Method
dvisc	0.0001185	Pa×s	922.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406008&Units=SI
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

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