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

Inchi: InChI=1S/C26H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-28-26(27)25-22-24(25)23

InchiKey: XYYLNWASRLMQKZ-UHFFFAOYSA-N

Formula: C26H42O2

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 386.61

Physical Properties

Property code	Value	Unit	Source
gf	99.57	kJ/mol	Joback Method
hf	-535.78	kJ/mol	Joback Method
hfus	59.13	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-8.29		Crippen Method
logp	7.815		Crippen Method
mcvol	350.020	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
rinpol	2965.00		NIST Webbook
rinpol	2965.00		NIST Webbook
tb	899.32	K	Joback Method
tc	1103.22	K	Joback Method
tf	495.06	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.98	J/mol×K	899.32	Joback Method
cpg	1269.09	J/mol×K	1069.24	Joback Method
cpg	1253.40	J/mol×K	1035.26	Joback Method
cpg	1236.73	J/mol×K	1001.27	Joback Method
cpg	1218.99	J/mol×K	967.29	Joback Method
cpg	1200.09	J/mol×K	933.30	Joback Method
cpg	1283.86	J/mol×K	1103.22	Joback Method
dvisc	0.0001346	Pa×s	899.32	Joback Method

dvisc	0.0001670	Pa×s	831.94	Joback Method
dvisc	0.0002152	Pa×s	764.57	Joback Method
dvisc	0.0002914	Pa×s	697.19	Joback Method
dvisc	0.0004209	Pa×s	629.81	Joback Method
dvisc	0.0006640	Pa×s	562.44	Joback Method
dvisc	0.0011860	Pa×s	495.06	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=U406007&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