cis-Cyclohex-4-en-1,2-dicarboxylic acid, 3-phenylpropyl undecyl ester

Inchi: InChI=1S/C28H42O4/c1-2-3-4-5-6-7-8-9-15-22-31-27(29)25-20-13-14-21-26(25)28(30)32

InchiKey: JPMLMNGXIXYMDR-UHFFFAOYSA-N

Formula: C28H42O4

SMILES: CCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 442.63

Physical Properties

Property code	Value	Unit	Source
gf	-123.85	kJ/mol	Joback Method
hf	-782.56	kJ/mol	Joback Method
hfus	62.02	kJ/mol	Joback Method
hvap	98.92	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.819		Crippen Method
mcvol	381.340	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	3228.00		NIST Webbook
rinpol	3228.00		NIST Webbook
tb	1033.34	K	Joback Method
tc	1265.11	K	Joback Method
tf	579.96	K	Joback Method
vc	1.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1336.43	J/mol×K	1033.34	Joback Method
cpg	1399.98	J/mol×K	1226.48	Joback Method
cpg	1390.71	J/mol×K	1187.85	Joback Method
cpg	1379.79	J/mol×K	1149.23	Joback Method
cpg	1367.15	J/mol×K	1110.60	Joback Method
cpg	1352.72	J/mol×K	1071.97	Joback Method
cpg	1407.68	J/mol×K	1265.11	Joback Method
dvisc	0.0000250	Pa×s	1033.34	Joback Method

dvisc	0.0000326	Pa×s	957.78	Joback Method
dvisc	0.0000446	Pa×s	882.21	Joback Method
dvisc	0.0000646	Pa×s	806.65	Joback Method
dvisc	0.0001011	Pa×s	731.09	Joback Method
dvisc	0.0001756	Pa×s	655.52	Joback Method
dvisc	0.0003519	Pa×s	579.96	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=U382782&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