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

Inchi: InChI=1S/C24H42O4/c1-3-5-7-8-9-10-11-12-16-20-28-24(26)22-18-14-13-17-21(22)23(2

InchiKey: AGRBZQVWKWDZTH-UHFFFAOYSA-N

Formula: C24H42O4

SMILES: CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCC

Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-269.94	kJ/mol	Joback Method
hf	-936.53	kJ/mol	Joback Method
hfus	57.62	kJ/mol	Joback Method
hvap	87.74	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.376		Crippen Method
mcvol	348.740	ml/mol	McGowan Method
pc	963.27	kPa	Joback Method
rinpol	2688.00		NIST Webbook
rinpol	2688.00		NIST Webbook
tb	915.14	K	Joback Method
tc	1120.90	K	Joback Method
tf	508.46	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.64	J/mol×K	915.14	Joback Method
cpg	1268.77	J/mol×K	1086.61	Joback Method
cpg	1255.71	J/mol×K	1052.31	Joback Method
cpg	1241.20	J/mol×K	1018.02	Joback Method
cpg	1225.21	J/mol×K	983.73	Joback Method
cpg	1207.70	J/mol×K	949.43	Joback Method
cpg	1280.40	J/mol×K	1120.90	Joback Method
dvisc	0.0000434	Pa×s	915.14	Joback Method

dvisc	0.0000569	Pa×s	847.36	Joback Method
dvisc	0.0000781	Pa×s	779.58	Joback Method
dvisc	0.0001139	Pa×s	711.80	Joback Method
dvisc	0.0001798	Pa×s	644.02	Joback Method
dvisc	0.0003160	Pa×s	576.24	Joback Method
dvisc	0.0006454	Pa×s	508.46	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=U382754&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