1,2-Cyclohexanedicarboxylic acid, cyclohex-3-enylmethyl undecyl ester

Inchi: InChI=1S/C26H44O4/c1-2-3-4-5-6-7-8-9-15-20-29-25(27)23-18-13-14-19-24(23)26(28)30
InchiKey: HOVDZITVMZCHEX-UHFFFAOYSA-N
Formula: C26H44O4
SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CC=CCC1
Mol. weight [g/mol]: 420.63

Physical Properties

Property code	Value	Unit	Source
gf	-228.65	kJ/mol	Joback Method
hf	-923.49	kJ/mol	Joback Method
hfus	54.63	kJ/mol	Joback Method
hvap	92.62	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.766		Crippen Method
mcvol	366.060	ml/mol	McGowan Method
pc	971.09	kPa	Joback Method
rinpol	3031.00		NIST Webbook
tb	980.45	K	Joback Method
tc	1201.49	K	Joback Method
tf	538.38	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1311.18	J/mol×K	980.45	Joback Method
cpg	1384.59	J/mol×K	1164.65	Joback Method
cpg	1373.62	J/mol×K	1127.81	Joback Method
cpg	1360.84	J/mol×K	1090.97	Joback Method
cpg	1346.21	J/mol×K	1054.13	Joback Method
cpg	1329.67	J/mol×K	1017.29	Joback Method
cpg	1393.81	J/mol×K	1201.49	Joback Method
dvisc	0.0000333	Pa×s	980.45	Joback Method
dvisc	0.0000442	Pa×s	906.77	Joback Method

dvisc	0.0000615	Pa×s	833.09	Joback Method
dvisc	0.0000914	Pa×s	759.41	Joback Method
dvisc	0.0001479	Pa×s	685.74	Joback Method
dvisc	0.0002687	Pa×s	612.06	Joback Method
dvisc	0.0005748	Pa×s	538.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339873&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

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