1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl undecyl ester

Inchi: InChI=1S/C26H46O4/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: WKLDKJRWDADVLJ-UHFFFAOYSA-N

Formula: C26H46O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1

Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-258.61	kJ/mol	Joback Method
hf	-981.27	kJ/mol	Joback Method
hfus	53.41	kJ/mol	Joback Method
hvap	92.33	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.990		Crippen Method
mcvol	370.360	ml/mol	McGowan Method
pc	949.67	kPa	Joback Method
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook
tb	981.29	K	Joback Method
tc	1202.24	K	Joback Method
tf	537.62	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1342.58	J/mol×K	981.29	Joback Method
cpg	1361.68	J/mol×K	1018.12	Joback Method
cpg	1378.76	J/mol×K	1054.94	Joback Method
cpg	1393.87	J/mol×K	1091.77	Joback Method
cpg	1407.05	J/mol×K	1128.59	Joback Method
cpg	1418.36	J/mol×K	1165.42	Joback Method
cpg	1427.85	J/mol×K	1202.24	Joback Method
dvisc	0.0005747	Pa×s	537.62	Joback Method

dvisc	0.0002618	Pa×s	611.57	Joback Method
dvisc	0.0001413	Pa×s	685.51	Joback Method
dvisc	0.0000860	Pa×s	759.45	Joback Method
dvisc	0.0000572	Pa×s	833.40	Joback Method
dvisc	0.0000406	Pa×s	907.35	Joback Method
dvisc	0.0000304	Pa×s	981.29	Joback Method

Sources

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=U339745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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