1,2-Cyclohexanedicarboxylic acid, 2-methylbutyl undecyl ester

Inchi: InChI=1S/C24H44O4/c1-4-6-7-8-9-10-11-12-15-18-27-23(25)21-16-13-14-17-22(21)24(2

InchiKey: LOLIHPPQIQCYRT-UHFFFAOYSA-N

Formula: C24H44O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)CC

Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-302.34	kJ/mol	Joback Method
hf	-999.59	kJ/mol	Joback Method
hfus	52.87	kJ/mol	Joback Method
hvap	87.06	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.456		Crippen Method
mcvol	353.040	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	2687.00		NIST Webbook
rinpol	2687.00		NIST Webbook
tb	915.54	K	Joback Method
tc	1121.60	K	Joback Method
tf	492.70	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1219.15	J/mol×K	915.54	Joback Method
cpg	1238.90	J/mol×K	949.88	Joback Method
cpg	1257.03	J/mol×K	984.23	Joback Method
cpg	1273.57	J/mol×K	1018.57	Joback Method
cpg	1288.55	J/mol×K	1052.92	Joback Method
cpg	1302.00	J/mol×K	1087.26	Joback Method
cpg	1313.95	J/mol×K	1121.60	Joback Method
dvisc	0.0007458	Pa×s	492.70	Joback Method

dvisc	0.0003291	Pa×s	563.17	Joback Method
dvisc	0.0001742	Pa×s	633.65	Joback Method
dvisc	0.0001047	Pa×s	704.12	Joback Method
dvisc	0.0000691	Pa×s	774.59	Joback Method
dvisc	0.0000488	Pa×s	845.07	Joback Method
dvisc	0.0000364	Pa×s	915.54	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=U339550&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