1,2-Cyclohexanedicarboxylic acid, 3-methylbut-2-yl undecyl ester

Inchi: InChI=1S/C24H44O4/c1-5-6-7-8-9-10-11-12-15-18-27-23(25)21-16-13-14-17-22(21)24(2

InchiKey: YFNMYKRTSXUWEE-UHFFFAOYSA-N

Formula: C24H44O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-304.78	kJ/mol	Joback Method
hf	-1004.87	kJ/mol	Joback Method
hfus	49.35	kJ/mol	Joback Method
hvap	86.67	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.454		Crippen Method
mcvol	353.040	ml/mol	McGowan Method
pc	951.42	kPa	Joback Method
rinpol	2645.00		NIST Webbook
tb	915.10	K	Joback Method
tc	1121.60	K	Joback Method
tf	477.70	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1219.56	J/mol×K	915.10	Joback Method
cpg	1239.32	J/mol×K	949.52	Joback Method
cpg	1257.45	J/mol×K	983.93	Joback Method
cpg	1273.97	J/mol×K	1018.35	Joback Method
cpg	1288.91	J/mol×K	1052.77	Joback Method
cpg	1302.30	J/mol×K	1087.18	Joback Method
cpg	1314.18	J/mol×K	1121.60	Joback Method
dvisc	0.0008669	Pa×s	477.70	Joback Method
dvisc	0.0003513	Pa×s	550.60	Joback Method

dvisc	0.0001758	Pa×s	623.50	Joback Method
dvisc	0.0001017	Pa×s	696.40	Joback Method
dvisc	0.0000653	Pa×s	769.30	Joback Method
dvisc	0.0000452	Pa×s	842.20	Joback Method
dvisc	0.0000332	Pa×s	915.10	Joback Method

Sources

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=U339564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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