1,2-Cyclohexanedicarboxylic acid, cyclohexyl undecyl ester

Inchi: InChI=1S/C25H44O4/c1-2-3-4-5-6-7-8-9-15-20-28-24(26)22-18-13-14-19-23(22)25(27)29

InchiKey: HMLMOHNYCAVDPR-UHFFFAOYSA-N

Formula: C25H44O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-267.03	kJ/mol	Joback Method
hf	-960.63	kJ/mol	Joback Method
hfus	50.82	kJ/mol	Joback Method
hvap	90.11	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.743		Crippen Method
mcvol	356.270	ml/mol	McGowan Method
pc	1008.45	kPa	Joback Method
rinpol	2904.00		NIST Webbook
rinpol	2904.00		NIST Webbook
tb	958.41	K	Joback Method
tc	1176.05	K	Joback Method
tf	526.35	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1279.03	J/mol×K	958.41	Joback Method
cpg	1298.29	J/mol×K	994.68	Joback Method
cpg	1315.61	J/mol×K	1030.96	Joback Method
cpg	1331.03	J/mol×K	1067.23	Joback Method
cpg	1344.60	J/mol×K	1103.50	Joback Method
cpg	1356.36	J/mol×K	1139.78	Joback Method
cpg	1366.35	J/mol×K	1176.05	Joback Method
dvisc	0.0006516	Pa×s	526.35	Joback Method

dvisc	0.0002993	Pa×s	598.36	Joback Method
dvisc	0.0001625	Pa×s	670.37	Joback Method
dvisc	0.0000994	Pa×s	742.38	Joback Method
dvisc	0.0000663	Pa×s	814.39	Joback Method
dvisc	0.0000472	Pa×s	886.40	Joback Method
dvisc	0.0000354	Pa×s	958.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339765&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

Latest version available from:
https://www.chemeo.com/cid/95-460-6/1-2-Cyclohexanedicarboxylic-acid-cyclohexyl-undecyl-ester.pdf
Generated by Cheméo on 2024-10-12 07:58:41.823649319 +0000 UTC m=+3300784.460618570.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.