1,2-Cyclohexanedicarboxylic acid, 2-methylcyclohexyl tetradecyl ester

Inchi: InChI=1S/C29H52O4/c1-3-4-5-6-7-8-9-10-11-12-13-18-23-32-28(30)25-20-15-16-21-26(2

InchiKey: CJGBNZHINCEPFU-UHFFFAOYSA-N

Formula: C29H52O4

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-241.06	kJ/mol	Joback Method
hf	-1063.53	kJ/mol	Joback Method
hfus	62.25	kJ/mol	Joback Method
hvap	98.70	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.159		Crippen Method
mcvol	412.630	ml/mol	McGowan Method
pc	786.39	kPa	Joback Method
rinpol	3264.00		NIST Webbook
rinpol	3264.00		NIST Webbook
tb	1045.26	K	Joback Method
tc	1281.08	K	Joback Method
tf	567.19	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1538.68	J/mol×K	1045.26	Joback Method
cpg	1557.42	J/mol×K	1084.56	Joback Method
cpg	1573.71	J/mol×K	1123.87	Joback Method
cpg	1587.59	J/mol×K	1163.17	Joback Method
cpg	1599.14	J/mol×K	1202.48	Joback Method
cpg	1608.42	J/mol×K	1241.78	Joback Method
cpg	1615.49	J/mol×K	1281.08	Joback Method
dvisc	0.0004472	Pa×s	567.19	Joback Method

dvisc	0.0002077	Pa×s	646.87	Joback Method
dvisc	0.0001142	Pa×s	726.55	Joback Method
dvisc	0.0000706	Pa×s	806.22	Joback Method
dvisc	0.0000476	Pa×s	885.90	Joback Method
dvisc	0.0000343	Pa×s	965.58	Joback Method
dvisc	0.0000259	Pa×s	1045.26	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=U339883&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