1,2-Cyclohexanedicarboxylic acid, 5-methoxy-3-methylpentyl tetradecyl ester

Inchi: InChI=1S/C29H54O5/c1-4-5-6-7-8-9-10-11-12-13-14-17-22-33-28(30)26-18-15-16-19-27

InchiKey: IATSOPYJXPEVGI-UHFFFAOYSA-N

Formula: C29H54O5

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 482.74

Physical Properties

Property code	Value	Unit	Source
gf	-365.24	kJ/mol	Joback Method
hf	-1235.01	kJ/mol	Joback Method
hfus	67.01	kJ/mol	Joback Method
hvap	100.60	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	7.643		Crippen Method
mcvol	429.360	ml/mol	McGowan Method
pc	712.25	kPa	Joback Method
rinpol	3287.00		NIST Webbook
tb	1052.36	K	Joback Method
tc	1300.80	K	Joback Method
tf	571.28	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1569.81	J/mol×K	1052.36	Joback Method
cpg	1641.08	J/mol×K	1259.39	Joback Method
cpg	1631.94	J/mol×K	1217.99	Joback Method
cpg	1620.30	J/mol×K	1176.58	Joback Method
cpg	1606.10	J/mol×K	1135.17	Joback Method
cpg	1589.29	J/mol×K	1093.77	Joback Method
cpg	1647.78	J/mol×K	1300.80	Joback Method
dvisc	0.0000124	Pa×s	1052.36	Joback Method
dvisc	0.0000167	Pa×s	972.18	Joback Method

dvisc	0.0000238	Pa×s	892.00	Joback Method
dvisc	0.0000362	Pa×s	811.82	Joback Method
dvisc	0.0000607	Pa×s	731.64	Joback Method
dvisc	0.0001152	Pa×s	651.46	Joback Method
dvisc	0.0002620	Pa×s	571.28	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=U339925&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