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

Inchi: InChI=1S/C27H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-18-21-30-26(28)24-19-16-17-20-2

InchiKey: UHXYNNFEIUIIRE-UHFFFAOYSA-N

Formula: C27H50O4

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

Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-279.52	kJ/mol	Joback Method
hf	-1066.79	kJ/mol	Joback Method
hfus	57.12	kJ/mol	Joback Method
hvap	93.35	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.625		Crippen Method
mcvol	395.310	ml/mol	McGowan Method
pc	802.51	kPa	Joback Method
rinpol	2952.00		NIST Webbook
rinpol	2952.00		NIST Webbook
tb	983.74	K	Joback Method
tc	1205.40	K	Joback Method
tf	511.51	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1411.04	J/mol×K	983.74	Joback Method
cpg	1492.39	J/mol×K	1168.46	Joback Method
cpg	1479.85	J/mol×K	1131.51	Joback Method
cpg	1465.49	J/mol×K	1094.57	Joback Method
cpg	1449.27	J/mol×K	1057.63	Joback Method
cpg	1431.14	J/mol×K	1020.68	Joback Method
cpg	1503.17	J/mol×K	1205.40	Joback Method
dvisc	0.0000210	Pa×s	983.74	Joback Method

dvisc	0.0000288	Pa×s	905.03	Joback Method
dvisc	0.0000418	Pa×s	826.33	Joback Method
dvisc	0.0000656	Pa×s	747.62	Joback Method
dvisc	0.0001145	Pa×s	668.92	Joback Method
dvisc	0.0002320	Pa×s	590.22	Joback Method
dvisc	0.0005841	Pa×s	511.51	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=U339566&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