1,2-Cyclohexanedicarboxylic acid, hexyl tetradecyl ester

Inchi: InChI=1S/C28H52O4/c1-3-5-7-9-10-11-12-13-14-15-16-20-24-32-28(30)26-22-18-17-21-

InchiKey: XJAOFGPMMGBRBI-UHFFFAOYSA-N

Formula: C28H52O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCC

Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-266.22	kJ/mol	Joback Method
hf	-1076.87	kJ/mol	Joback Method
hfus	66.76	kJ/mol	Joback Method
hvap	96.35	kJ/mol	Joback Method
log10ws	-8.68		Crippen Method
logp	8.161		Crippen Method
mcvol	409.400	ml/mol	McGowan Method
pc	753.91	kPa	Joback Method
rinpol	3141.00		NIST Webbook
rinpol	3141.00		NIST Webbook
tb	1007.50	K	Joback Method
tc	1238.90	K	Joback Method
tf	552.78	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.90	J/mol×K	1007.50	Joback Method
cpg	1495.49	J/mol×K	1046.07	Joback Method
cpg	1513.96	J/mol×K	1084.63	Joback Method
cpg	1530.36	J/mol×K	1123.20	Joback Method
cpg	1544.76	J/mol×K	1161.77	Joback Method
cpg	1557.22	J/mol×K	1200.34	Joback Method
cpg	1567.79	J/mol×K	1238.90	Joback Method
dvisc	0.0003982	Pa×s	552.78	Joback Method

dvisc	0.0001832	Pa×s	628.57	Joback Method
dvisc	0.0000996	Pa×s	704.35	Joback Method
dvisc	0.0000610	Pa×s	780.14	Joback Method
dvisc	0.0000407	Pa×s	855.93	Joback Method
dvisc	0.0000290	Pa×s	931.71	Joback Method
dvisc	0.0000218	Pa×s	1007.50	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=U339418&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