1,2-Cyclohexanedicarboxylic acid, pentyl tetradecyl ester

Inchi: InChI=1S/C27H50O4/c1-3-5-7-8-9-10-11-12-13-14-15-19-23-31-27(29)25-21-17-16-20-2
InchiKey: KGBLWMYBBFJATI-UHFFFAOYSA-N
Formula: C27H50O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-274.64	kJ/mol	Joback Method
hf	-1056.23	kJ/mol	Joback Method
hfus	64.17	kJ/mol	Joback Method
hvap	94.13	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.771		Crippen Method
mcvol	395.310	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	3062.00		NIST Webbook
rinpol	3062.00		NIST Webbook
tb	984.62	K	Joback Method
tc	1207.94	K	Joback Method
tf	541.51	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.41	J/mol×K	984.62	Joback Method
cpg	1430.75	J/mol×K	1021.84	Joback Method
cpg	1449.13	J/mol×K	1059.06	Joback Method
cpg	1465.59	J/mol×K	1096.28	Joback Method
cpg	1480.19	J/mol×K	1133.50	Joback Method
cpg	1492.98	J/mol×K	1170.72	Joback Method
cpg	1504.00	J/mol×K	1207.94	Joback Method
dvisc	0.0004525	Pa×s	541.51	Joback Method

dvisc	0.0002099	Pa×s	615.36	Joback Method
dvisc	0.0001148	Pa×s	689.21	Joback Method
dvisc	0.0000706	Pa×s	763.07	Joback Method
dvisc	0.0000473	Pa×s	836.92	Joback Method
dvisc	0.0000338	Pa×s	910.77	Joback Method
dvisc	0.0000254	Pa×s	984.62	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=U339476&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