1,2-Cyclohexanedicarboxylic acid, 4-octyl tetradecyl ester

Inchi: InChI=1S/C30H56O4/c1-4-7-9-10-11-12-13-14-15-16-17-20-25-33-29(31)27-23-18-19-24

InchiKey: PPQURVWPTQIGNM-UHFFFAOYSA-N

Formula: C30H56O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CCC)CCCC

Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-251.82	kJ/mol	Joback Method
hf	-1123.43	kJ/mol	Joback Method
hfus	68.41	kJ/mol	Joback Method
hvap	100.42	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	8.939		Crippen Method
mcvol	437.580	ml/mol	McGowan Method
pc	683.14	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	1052.82	K	Joback Method
tc	1301.97	K	Joback Method
tf	560.32	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.69	J/mol×K	1052.82	Joback Method
cpg	1625.59	J/mol×K	1094.35	Joback Method
cpg	1643.99	J/mol×K	1135.87	Joback Method
cpg	1659.98	J/mol×K	1177.40	Joback Method
cpg	1673.65	J/mol×K	1218.92	Joback Method
cpg	1685.07	J/mol×K	1260.45	Joback Method
cpg	1694.33	J/mol×K	1301.97	Joback Method
dvisc	0.0003411	Pa×s	560.32	Joback Method

dvisc	0.0001438	Pa×s	642.40	Joback Method
dvisc	0.0000738	Pa×s	724.49	Joback Method
dvisc	0.0000433	Pa×s	806.57	Joback Method
dvisc	0.0000281	Pa×s	888.65	Joback Method
dvisc	0.0000196	Pa×s	970.74	Joback Method
dvisc	0.0000145	Pa×s	1052.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339528&Units=SI
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

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