1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl pentadecyl ester

Inchi: InChI=1S/C31H56O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-25-34-30(32)28-22-17-18-23-29

InchiKey: HBNCTFWCYBBOHZ-UHFFFAOYSA-N

Formula: C31H56O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
gf	-216.51	kJ/mol	Joback Method
hf	-1084.47	kJ/mol	Joback Method
hfus	66.36	kJ/mol	Joback Method
hvap	103.46	kJ/mol	Joback Method
log10ws	-9.59		Crippen Method
logp	8.941		Crippen Method
mcvol	440.810	ml/mol	McGowan Method
pc	720.69	kPa	Joback Method
rinpol	3546.00		NIST Webbook
rinpol	3546.00		NIST Webbook
tb	1095.69	K	Joback Method
tc	1349.57	K	Joback Method
tf	593.97	K	Joback Method
vc	1.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1662.99	J/mol×K	1095.69	Joback Method
cpg	1681.56	J/mol×K	1138.00	Joback Method
cpg	1697.42	J/mol×K	1180.32	Joback Method
cpg	1710.69	J/mol×K	1222.63	Joback Method
cpg	1721.44	J/mol×K	1264.95	Joback Method
cpg	1729.80	J/mol×K	1307.26	Joback Method
cpg	1735.85	J/mol×K	1349.57	Joback Method
dvisc	0.0002953	Pa×s	593.97	Joback Method

dvisc	0.0001295	Pa×s	677.59	Joback Method
dvisc	0.0000681	Pa×s	761.21	Joback Method
dvisc	0.0000406	Pa×s	844.83	Joback Method
dvisc	0.0000266	Pa×s	928.45	Joback Method
dvisc	0.0000187	Pa×s	1012.07	Joback Method
dvisc	0.0000139	Pa×s	1095.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339734&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

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