1,2-Cyclohexanedicarboxylic acid, 2-methylpent-3-yl octadecyl ester

Inchi: InChI=1S/C32H60O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-26-35-31(33)28-

InchiKey: DZCLNEKLTHOLGB-UHFFFAOYSA-N

Formula: C32H60O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 508.82

Physical Properties

Property code	Value	Unit	Source
gf	-237.42	kJ/mol	Joback Method
hf	-1169.99	kJ/mol	Joback Method
hfus	70.07	kJ/mol	Joback Method
hvap	104.48	kJ/mol	Joback Method
log10ws	-10.22		Crippen Method
logp	9.575		Crippen Method
mcvol	465.760	ml/mol	McGowan Method
pc	621.89	kPa	Joback Method
rinpol	3562.00		NIST Webbook
rinpol	3562.00		NIST Webbook
tb	1098.14	K	Joback Method
tc	1368.93	K	Joback Method
tf	567.86	K	Joback Method
vc	1.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1734.82	J/mol×K	1098.14	Joback Method
cpg	1812.00	J/mol×K	1323.80	Joback Method
cpg	1802.00	J/mol×K	1278.67	Joback Method
cpg	1789.40	J/mol×K	1233.53	Joback Method
cpg	1774.09	J/mol×K	1188.40	Joback Method
cpg	1755.93	J/mol×K	1143.27	Joback Method
cpg	1819.54	J/mol×K	1368.93	Joback Method
dvisc	0.0000095	Pa×s	1098.14	Joback Method

dvisc	0.0000131	Pa×s	1009.76	Joback Method
dvisc	0.0000192	Pa×s	921.38	Joback Method
dvisc	0.0000305	Pa×s	833.00	Joback Method
dvisc	0.0000540	Pa×s	744.62	Joback Method
dvisc	0.0001115	Pa×s	656.24	Joback Method
dvisc	0.0002887	Pa×s	567.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339451&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