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

Inchi: InChI=1S/C30H54O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-24-33-29(31)26-21-16-17-22-2

InchiKey: SSPGLHMSECSKSB-UHFFFAOYSA-N

Formula: C30H54O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 478.75

Physical Properties

Property code	Value	Unit	Source
gf	-232.64	kJ/mol	Joback Method
hf	-1084.17	kJ/mol	Joback Method
hfus	64.84	kJ/mol	Joback Method
hvap	100.93	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	8.549		Crippen Method
mcvol	426.720	ml/mol	McGowan Method
pc	745.70	kPa	Joback Method
rinpol	3370.00		NIST Webbook
rinpol	3370.00		NIST Webbook
tb	1068.14	K	Joback Method
tc	1311.51	K	Joback Method
tf	578.46	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1602.89	J/mol×K	1068.14	Joback Method
cpg	1670.26	J/mol×K	1270.95	Joback Method
cpg	1661.75	J/mol×K	1230.39	Joback Method
cpg	1650.83	J/mol×K	1189.83	Joback Method
cpg	1637.43	J/mol×K	1149.26	Joback Method
cpg	1621.48	J/mol×K	1108.70	Joback Method
cpg	1676.44	J/mol×K	1311.51	Joback Method
dvisc	0.0000223	Pa×s	1068.14	Joback Method

dvisc	0.0000295	Pa×s	986.53	Joback Method
dvisc	0.0000410	Pa×s	904.91	Joback Method
dvisc	0.0000610	Pa×s	823.30	Joback Method
dvisc	0.0000991	Pa×s	741.69	Joback Method
dvisc	0.0001814	Pa×s	660.07	Joback Method
dvisc	0.0003936	Pa×s	578.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339884&Units=SI

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