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

Inchi: InChI=1S/C30H54O4/c1-2-3-4-5-6-7-8-9-10-11-12-18-24-33-29(31)27-21-16-17-22-28(27

InchiKey: JOKNBIUQXMHWFA-UHFFFAOYSA-N

Formula: C30H54O4

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

Mol. weight [g/mol]: 478.75

Physical Properties

Property code	Value	Unit	Source
gf	-224.93	kJ/mol	Joback Method
hf	-1063.83	kJ/mol	Joback Method
hfus	63.77	kJ/mol	Joback Method
hvap	101.23	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	8.551		Crippen Method
mcvol	426.720	ml/mol	McGowan Method
pc	759.32	kPa	Joback Method
rinpol	3431.00		NIST Webbook
rinpol	3431.00		NIST Webbook
tb	1072.81	K	Joback Method
tc	1317.67	K	Joback Method
tf	582.70	K	Joback Method
vc	1.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1598.70	J/mol×K	1072.81	Joback Method
cpg	1667.56	J/mol×K	1276.86	Joback Method
cpg	1658.49	J/mol×K	1236.05	Joback Method
cpg	1647.15	J/mol×K	1195.24	Joback Method
cpg	1633.46	J/mol×K	1154.43	Joback Method
cpg	1617.34	J/mol×K	1113.62	Joback Method
cpg	1674.45	J/mol×K	1317.67	Joback Method
dvisc	0.0000163	Pa×s	1072.81	Joback Method

dvisc	0.0000219	Pa×s	991.12	Joback Method
dvisc	0.0000311	Pa×s	909.44	Joback Method
dvisc	0.0000474	Pa×s	827.75	Joback Method
dvisc	0.0000791	Pa×s	746.07	Joback Method
dvisc	0.0001497	Pa×s	664.38	Joback Method
dvisc	0.0003389	Pa×s	582.70	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=U339733&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