1,2-Cyclohexanedicarboxylic acid, hexadecyl 2-methylbutyl ester

Inchi: InChI=1S/C29H54O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-20-23-32-28(30)26-21-18-1

InchiKey: ZAXSDNAEFZNOQN-UHFFFAOYSA-N

Formula: C29H54O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)CC

Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-260.24	kJ/mol	Joback Method
hf	-1102.79	kJ/mol	Joback Method
hfus	65.82	kJ/mol	Joback Method
hvap	98.19	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.407		Crippen Method
mcvol	423.490	ml/mol	McGowan Method
pc	718.76	kPa	Joback Method
rinpol	3219.00		NIST Webbook
rinpol	3219.00		NIST Webbook
tb	1029.94	K	Joback Method
tc	1268.88	K	Joback Method
tf	549.05	K	Joback Method
vc	1.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.85	J/mol×K	1029.94	Joback Method
cpg	1620.87	J/mol×K	1229.05	Joback Method
cpg	1608.96	J/mol×K	1189.23	Joback Method
cpg	1594.98	J/mol×K	1149.41	Joback Method
cpg	1578.85	J/mol×K	1109.59	Joback Method
cpg	1560.50	J/mol×K	1069.76	Joback Method
cpg	1630.76	J/mol×K	1268.88	Joback Method
dvisc	0.0000169	Pa×s	1029.94	Joback Method

dvisc	0.0000229	Pa×s	949.79	Joback Method
dvisc	0.0000328	Pa×s	869.64	Joback Method
dvisc	0.0000504	Pa×s	789.50	Joback Method
dvisc	0.0000856	Pa×s	709.35	Joback Method
dvisc	0.0001660	Pa×s	629.20	Joback Method
dvisc	0.0003910	Pa×s	549.05	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=U339554&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