1,2-Cyclohexanedicarboxylic acid, hexadecyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C29H54O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-32-28(30)26-21-18-1

InchiKey: QVWVBWUZRNSUHV-UHFFFAOYSA-N

Formula: C29H54O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-262.68	kJ/mol	Joback Method
hf	-1108.07	kJ/mol	Joback Method
hfus	62.30	kJ/mol	Joback Method
hvap	97.80	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	8.405		Crippen Method
mcvol	423.490	ml/mol	McGowan Method
pc	721.85	kPa	Joback Method
rinpol	3169.00		NIST Webbook
rinpol	3169.00		NIST Webbook
tb	1029.50	K	Joback Method
tc	1266.79	K	Joback Method
tf	534.05	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.09	J/mol×K	1029.50	Joback Method
cpg	1560.53	J/mol×K	1069.05	Joback Method
cpg	1578.69	J/mol×K	1108.60	Joback Method
cpg	1594.64	J/mol×K	1148.14	Joback Method
cpg	1608.46	J/mol×K	1187.69	Joback Method
cpg	1620.21	J/mol×K	1227.24	Joback Method
cpg	1629.96	J/mol×K	1266.79	Joback Method
dvisc	0.0004434	Pa×s	534.05	Joback Method

dvisc	0.0001740	Pa×s	616.62	Joback Method
dvisc	0.0000852	Pa×s	699.20	Joback Method
dvisc	0.0000485	Pa×s	781.77	Joback Method
dvisc	0.0000307	Pa×s	864.35	Joback Method
dvisc	0.0000211	Pa×s	946.92	Joback Method
dvisc	0.0000154	Pa×s	1029.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339568&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