1,2-Cyclohexanedicarboxylic acid, dodecyl 5-methoxy-3-methylpentyl ester

Inchi: InChI=1S/C27H50O5/c1-4-5-6-7-8-9-10-11-12-15-20-31-26(28)24-16-13-14-17-25(24)27

InchiKey: KVDGRLIOUVXURV-UHFFFAOYSA-N

Formula: C27H50O5

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 454.68

Physical Properties

Property code	Value	Unit	Source
gf	-382.08	kJ/mol	Joback Method
hf	-1193.73	kJ/mol	Joback Method
hfus	61.83	kJ/mol	Joback Method
hvap	96.15	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.863		Crippen Method
mcvol	401.180	ml/mol	McGowan Method
pc	791.26	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	1006.60	K	Joback Method
tc	1236.22	K	Joback Method
tf	548.74	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.65	J/mol×K	1006.60	Joback Method
cpg	1460.93	J/mol×K	1044.87	Joback Method
cpg	1477.97	J/mol×K	1083.14	Joback Method
cpg	1492.81	J/mol×K	1121.41	Joback Method
cpg	1505.49	J/mol×K	1159.68	Joback Method
cpg	1516.05	J/mol×K	1197.95	Joback Method
cpg	1524.51	J/mol×K	1236.22	Joback Method
dvisc	0.0003430	Pa×s	548.74	Joback Method

dvisc	0.0001531	Pa×s	625.05	Joback Method
dvisc	0.0000814	Pa×s	701.36	Joback Method
dvisc	0.0000490	Pa×s	777.67	Joback Method
dvisc	0.0000323	Pa×s	853.98	Joback Method
dvisc	0.0000228	Pa×s	930.29	Joback Method
dvisc	0.0000170	Pa×s	1006.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339924&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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