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

Inchi: InChI=1S/C24H44O5/c1-4-5-6-7-8-9-12-17-28-23(25)21-13-10-11-14-22(21)24(26)29-19

InchiKey: DYGUYTBAAFXSKJ-UHFFFAOYSA-N

Formula: C24H44O5

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

Mol. weight [g/mol]: 412.60

Physical Properties

Property code	Value	Unit	Source
gf	-407.34	kJ/mol	Joback Method
hf	-1131.81	kJ/mol	Joback Method
hfus	54.06	kJ/mol	Joback Method
hvap	89.47	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.692		Crippen Method
mcvol	358.910	ml/mol	McGowan Method
pc	936.92	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	937.96	K	Joback Method
tc	1148.38	K	Joback Method
tf	514.93	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.88	J/mol×K	937.96	Joback Method
cpg	1328.30	J/mol×K	1113.31	Joback Method
cpg	1316.32	J/mol×K	1078.24	Joback Method
cpg	1302.61	J/mol×K	1043.17	Joback Method
cpg	1287.15	J/mol×K	1008.10	Joback Method
cpg	1269.91	J/mol×K	973.03	Joback Method
cpg	1338.57	J/mol×K	1148.38	Joback Method
dvisc	0.0000270	Pa×s	937.96	Joback Method

dvisc	0.0000360	Pa×s	867.45	Joback Method
dvisc	0.0000507	Pa×s	796.95	Joback Method
dvisc	0.0000761	Pa×s	726.44	Joback Method
dvisc	0.0001248	Pa×s	655.94	Joback Method
dvisc	0.0002306	Pa×s	585.43	Joback Method
dvisc	0.0005041	Pa×s	514.93	Joback Method

Sources

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=U339921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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