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

Inchi: InChI=1S/C26H48O5/c1-4-5-6-7-8-9-10-11-14-19-30-25(27)23-15-12-13-16-24(23)26(28

InchiKey: WHCYEAZBSAJJNU-UHFFFAOYSA-N

Formula: C26H48O5

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

Mol. weight [g/mol]: 440.66

Physical Properties

Property code	Value	Unit	Source
gf	-390.50	kJ/mol	Joback Method
hf	-1173.09	kJ/mol	Joback Method
hfus	59.24	kJ/mol	Joback Method
hvap	93.92	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.473		Crippen Method
mcvol	387.090	ml/mol	McGowan Method
pc	835.79	kPa	Joback Method
rinpol	2973.00		NIST Webbook
rinpol	2973.00		NIST Webbook
tb	983.72	K	Joback Method
tc	1205.82	K	Joback Method
tf	537.47	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.81	J/mol×K	983.72	Joback Method
cpg	1397.00	J/mol×K	1020.74	Joback Method
cpg	1414.12	J/mol×K	1057.75	Joback Method
cpg	1429.20	J/mol×K	1094.77	Joback Method
cpg	1442.28	J/mol×K	1131.79	Joback Method
cpg	1453.39	J/mol×K	1168.81	Joback Method
cpg	1462.55	J/mol×K	1205.82	Joback Method
dvisc	0.0003910	Pa×s	537.47	Joback Method

dvisc	0.0001759	Pa×s	611.85	Joback Method
dvisc	0.0000941	Pa×s	686.22	Joback Method
dvisc	0.0000569	Pa×s	760.60	Joback Method
dvisc	0.0000376	Pa×s	834.97	Joback Method
dvisc	0.0000266	Pa×s	909.35	Joback Method
dvisc	0.0000198	Pa×s	983.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339923&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