1,2-Cyclohexanedicarboxylic acid, dodecyl furfuryl ester

Inchi: InChI=1S/C25H44O5/c1-2-3-4-5-6-7-8-9-10-13-18-29-24(26)22-16-11-12-17-23(22)25(27

InchiKey: SSQGHXDPRBSVHN-UHFFFAOYSA-N

Formula: C25H44O5

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCO1

Mol. weight [g/mol]: 424.61

Physical Properties

Property code	Value	Unit	Source
gf	-341.05	kJ/mol	Joback Method
hf	-1086.47	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	94.44	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.979		Crippen Method
mcvol	362.140	ml/mol	McGowan Method
pc	987.02	kPa	Joback Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook
tb	981.09	K	Joback Method
tc	1201.49	K	Joback Method
tf	556.44	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.96	J/mol×K	981.09	Joback Method
cpg	1327.41	J/mol×K	1017.82	Joback Method
cpg	1343.98	J/mol×K	1054.56	Joback Method
cpg	1358.73	J/mol×K	1091.29	Joback Method
cpg	1371.71	J/mol×K	1128.02	Joback Method
cpg	1382.97	J/mol×K	1164.75	Joback Method
cpg	1392.55	J/mol×K	1201.49	Joback Method
dvisc	0.0006249	Pa×s	556.44	Joback Method

dvisc	0.0003126	Pa×s	627.22	Joback Method
dvisc	0.0001800	Pa×s	697.99	Joback Method
dvisc	0.0001147	Pa×s	768.77	Joback Method
dvisc	0.0000789	Pa×s	839.54	Joback Method
dvisc	0.0000575	Pa×s	910.32	Joback Method
dvisc	0.0000439	Pa×s	981.09	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=U339903&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