1,2-Cyclohexanedicarboxylic acid, furfuryl pentadecyl ester

Inchi: InChI=1S/C28H50O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-21-32-27(29)25-19-14-15-20-26

InchiKey: VNMFCFCXDJAVQN-UHFFFAOYSA-N

Formula: C28H50O5

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

Mol. weight [g/mol]: 466.69

Physical Properties

Property code	Value	Unit	Source
gf	-315.79	kJ/mol	Joback Method
hf	-1148.39	kJ/mol	Joback Method
hfus	68.67	kJ/mol	Joback Method
hvap	101.12	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.149		Crippen Method
mcvol	404.410	ml/mol	McGowan Method
pc	830.02	kPa	Joback Method
rinpol	3362.00		NIST Webbook
rinpol	3362.00		NIST Webbook
tb	1049.73	K	Joback Method
tc	1287.83	K	Joback Method
tf	590.25	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1499.81	J/mol×K	1049.73	Joback Method
cpg	1570.57	J/mol×K	1248.14	Joback Method
cpg	1560.54	J/mol×K	1208.46	Joback Method
cpg	1548.53	J/mol×K	1168.78	Joback Method
cpg	1534.46	J/mol×K	1129.10	Joback Method
cpg	1518.24	J/mol×K	1089.41	Joback Method
cpg	1578.69	J/mol×K	1287.83	Joback Method
dvisc	0.0000277	Pa×s	1049.73	Joback Method

dvisc	0.0000365	Pa×s	973.15	Joback Method
dvisc	0.0000505	Pa×s	896.57	Joback Method
dvisc	0.0000742	Pa×s	819.99	Joback Method
dvisc	0.0001181	Pa×s	743.41	Joback Method
dvisc	0.0002091	Pa×s	666.83	Joback Method
dvisc	0.0004293	Pa×s	590.25	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=U339905&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