1,2-Cyclohexanedicarboxylic acid, furfuryl octyl ester

Inchi: InChI=1S/C21H36O5/c1-2-3-4-5-6-9-14-25-20(22)18-12-7-8-13-19(18)21(23)26-16-17-11

InchiKey: QYTUZABTSGPWQH-UHFFFAOYSA-N

Formula: C21H36O5

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

Mol. weight [g/mol]: 368.51

Physical Properties

Property code	Value	Unit	Source
gf	-374.73	kJ/mol	Joback Method
hf	-1003.91	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	85.54	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.419		Crippen Method
mcvol	305.780	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2629.00		NIST Webbook
rinpol	2629.00		NIST Webbook
tb	889.57	K	Joback Method
tc	1100.29	K	Joback Method
tf	511.36	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.80	J/mol×K	889.57	Joback Method
cpg	1136.66	J/mol×K	1065.17	Joback Method
cpg	1124.20	J/mol×K	1030.05	Joback Method
cpg	1110.21	J/mol×K	994.93	Joback Method
cpg	1094.67	J/mol×K	959.81	Joback Method
cpg	1077.55	J/mol×K	924.69	Joback Method
cpg	1147.63	J/mol×K	1100.29	Joback Method
dvisc	0.0000790	Pa×s	889.57	Joback Method

dvisc	0.0001026	Pa×s	826.53	Joback Method
dvisc	0.0001389	Pa×s	763.50	Joback Method
dvisc	0.0001988	Pa×s	700.46	Joback Method
dvisc	0.0003052	Pa×s	637.43	Joback Method
dvisc	0.0005151	Pa×s	574.39	Joback Method
dvisc	0.0009887	Pa×s	511.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339901&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