1,2-Cyclohexanedicarboxylic acid, furfuryl pentyl ester

Inchi: InChI=1S/C18H30O5/c1-2-3-6-11-22-17(19)15-9-4-5-10-16(15)18(20)23-13-14-8-7-12-21

InchiKey: OVGAWYBUXLBPPX-UHFFFAOYSA-N

Formula: C18H30O5

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

Mol. weight [g/mol]: 326.43

Physical Properties

Property code	Value	Unit	Source
gf	-399.99	kJ/mol	Joback Method
hf	-941.99	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.248		Crippen Method
mcvol	263.510	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
tb	820.93	K	Joback Method
tc	1032.70	K	Joback Method
tf	477.55	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.36	J/mol×K	820.93	Joback Method
cpg	895.41	J/mol×K	856.23	Joback Method
cpg	912.95	J/mol×K	891.52	Joback Method
cpg	928.98	J/mol×K	926.82	Joback Method
cpg	943.54	J/mol×K	962.11	Joback Method
cpg	956.65	J/mol×K	997.41	Joback Method
cpg	968.33	J/mol×K	1032.70	Joback Method
dvisc	0.0013412	Pa×s	477.55	Joback Method

dvisc	0.0007232	Pa×s	534.78	Joback Method
dvisc	0.0004394	Pa×s	592.01	Joback Method
dvisc	0.0002915	Pa×s	649.24	Joback Method
dvisc	0.0002067	Pa×s	706.47	Joback Method
dvisc	0.0001543	Pa×s	763.70	Joback Method
dvisc	0.0001200	Pa×s	820.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339898&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