1,2-Cyclohexanedicarboxylic acid, furfuryl hexyl ester

Inchi: InChI=1S/C19H32O5/c1-2-3-4-7-12-23-18(20)16-10-5-6-11-17(16)19(21)24-14-15-9-8-13

InchiKey: TWKJAVBNEUCFRB-UHFFFAOYSA-N

Formula: C19H32O5

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

Mol. weight [g/mol]: 340.45

Physical Properties

Property code	Value	Unit	Source
gf	-391.57	kJ/mol	Joback Method
hf	-962.63	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	81.09	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.639		Crippen Method
mcvol	277.600	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook
tb	843.81	K	Joback Method
tc	1054.54	K	Joback Method
tf	488.82	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.56	J/mol×K	843.81	Joback Method
cpg	955.51	J/mol×K	878.93	Joback Method
cpg	972.92	J/mol×K	914.05	Joback Method
cpg	988.80	J/mol×K	949.18	Joback Method
cpg	1003.19	J/mol×K	984.30	Joback Method
cpg	1016.11	J/mol×K	1019.42	Joback Method
cpg	1027.58	J/mol×K	1054.54	Joback Method
dvisc	0.0012168	Pa×s	488.82	Joback Method

dvisc	0.0006483	Pa×s	547.99	Joback Method
dvisc	0.0003905	Pa×s	607.15	Joback Method
dvisc	0.0002574	Pa×s	666.31	Joback Method
dvisc	0.0001816	Pa×s	725.48	Joback Method
dvisc	0.0001350	Pa×s	784.64	Joback Method
dvisc	0.0001047	Pa×s	843.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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