1,2-Cyclohexanedicarboxylic acid, furfuryl heptyl ester

Inchi: InChI=1S/C20H34O5/c1-2-3-4-5-8-13-24-19(21)17-11-6-7-12-18(17)20(22)25-15-16-10-9

InchiKey: GQVIGEMIZLUMDV-UHFFFAOYSA-N

Formula: C20H34O5

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

Mol. weight [g/mol]: 354.48

Physical Properties

Property code	Value	Unit	Source
gf	-383.15	kJ/mol	Joback Method
hf	-983.27	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	83.31	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.029		Crippen Method
mcvol	291.690	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook
tb	866.69	K	Joback Method
tc	1077.06	K	Joback Method
tf	500.09	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.39	J/mol×K	866.69	Joback Method
cpg	1016.24	J/mol×K	901.75	Joback Method
cpg	1033.51	J/mol×K	936.81	Joback Method
cpg	1049.23	J/mol×K	971.87	Joback Method
cpg	1063.43	J/mol×K	1006.93	Joback Method
cpg	1076.13	J/mol×K	1042.00	Joback Method
cpg	1087.36	J/mol×K	1077.06	Joback Method
dvisc	0.0010991	Pa×s	500.09	Joback Method

dvisc	0.0005789	Pa×s	561.19	Joback Method
dvisc	0.0003458	Pa×s	622.29	Joback Method
dvisc	0.0002265	Pa×s	683.39	Joback Method
dvisc	0.0001591	Pa×s	744.49	Joback Method
dvisc	0.0001178	Pa×s	805.59	Joback Method
dvisc	0.0000911	Pa×s	866.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339900&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