1,2-Cyclohexanedicarboxylic acid, heptyl propyl ester

Inchi: InChI=1S/C18H32O4/c1-3-5-6-7-10-14-22-18(20)16-12-9-8-11-15(16)17(19)21-13-4-2/h1

InchiKey: UYSJKASHSPGJPV-UHFFFAOYSA-N

Formula: C18H32O4

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

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-350.42	kJ/mol	Joback Method
hf	-870.47	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.260		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	778.70	K	Joback Method
tc	973.21	K	Joback Method
tf	440.08	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.78	J/mol×K	778.70	Joback Method
cpg	867.82	J/mol×K	811.12	Joback Method
cpg	885.63	J/mol×K	843.54	Joback Method
cpg	902.23	J/mol×K	875.95	Joback Method
cpg	917.63	J/mol×K	908.37	Joback Method
cpg	931.83	J/mol×K	940.79	Joback Method
cpg	944.86	J/mol×K	973.21	Joback Method
dvisc	0.0012314	Pa×s	440.08	Joback Method

dvisc	0.0006262	Pa×s	496.52	Joback Method
dvisc	0.0003655	Pa×s	552.95	Joback Method
dvisc	0.0002358	Pa×s	609.39	Joback Method
dvisc	0.0001638	Pa×s	665.83	Joback Method
dvisc	0.0001205	Pa×s	722.26	Joback Method
dvisc	0.0000926	Pa×s	778.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339532&Units=SI

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