1,2-Cyclohexanedicarboxylic acid, hexyl octyl ester

Inchi: InChI=1S/C22H40O4/c1-3-5-7-9-10-14-18-26-22(24)20-16-12-11-15-19(20)21(23)25-17-

InchiKey: MYNDADASTAWLIU-UHFFFAOYSA-N

Formula: C22H40O4

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

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-316.74	kJ/mol	Joback Method
hf	-953.03	kJ/mol	Joback Method
hfus	51.22	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.820		Crippen Method
mcvol	324.860	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
tb	870.22	K	Joback Method
tc	1069.14	K	Joback Method
tf	485.16	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.02	J/mol×K	870.22	Joback Method
cpg	1112.49	J/mol×K	903.37	Joback Method
cpg	1130.52	J/mol×K	936.53	Joback Method
cpg	1147.13	J/mol×K	969.68	Joback Method
cpg	1162.35	J/mol×K	1002.83	Joback Method
cpg	1176.19	J/mol×K	1035.99	Joback Method
cpg	1188.68	J/mol×K	1069.14	Joback Method
dvisc	0.0008194	Pa×s	485.16	Joback Method

dvisc	0.0003983	Pa×s	549.34	Joback Method
dvisc	0.0002252	Pa×s	613.51	Joback Method
dvisc	0.0001418	Pa×s	677.69	Joback Method
dvisc	0.0000968	Pa×s	741.87	Joback Method
dvisc	0.0000702	Pa×s	806.04	Joback Method
dvisc	0.0000534	Pa×s	870.22	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=U339413&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