1,2-Cyclohexanedicarboxylic acid, diheptyl ester

Inchi: InChI=1S/C22H40O4/c1-3-5-7-9-13-17-25-21(23)19-15-11-12-16-20(19)22(24)26-18-14-

InchiKey: JYNJINSLEOLPPO-UHFFFAOYSA-N

Formula: C22H40O4

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

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	2517.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U339538&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