cis-Cyclohex-4-en-1,2-dicarboxylic acid, hexyl pentyl ester

Inchi: InChI=1S/C19H32O4/c1-3-5-7-11-15-23-19(21)17-13-9-8-12-16(17)18(20)22-14-10-6-4-2

InchiKey: KLVYOCASGORHKQ-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCC

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-312.04	kJ/mol	Joback Method
hf	-833.33	kJ/mol	Joback Method
hfus	44.67	kJ/mol	Joback Method
hvap	76.61	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.426		Crippen Method
mcvol	278.290	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tb	800.74	K	Joback Method
tc	996.12	K	Joback Method
tf	452.11	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.50	J/mol×K	800.74	Joback Method
cpg	899.89	J/mol×K	833.30	Joback Method
cpg	917.04	J/mol×K	865.87	Joback Method
cpg	932.98	J/mol×K	898.43	Joback Method
cpg	947.71	J/mol×K	931.00	Joback Method
cpg	961.26	J/mol×K	963.56	Joback Method
cpg	973.63	J/mol×K	996.12	Joback Method
dvisc	0.0010801	Pa×s	452.11	Joback Method

dvisc	0.0005587	Pa×s	510.22	Joback Method
dvisc	0.0003307	Pa×s	568.32	Joback Method
dvisc	0.0002158	Pa×s	626.42	Joback Method
dvisc	0.0001513	Pa×s	684.53	Joback Method
dvisc	0.0001122	Pa×s	742.63	Joback Method
dvisc	0.0000869	Pa×s	800.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382662&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

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