1,2-Cyclohexanedicarboxylic acid, cyclohexyl pentyl ester

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

InchiKey: QYHWQVQDFKZJAX-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-317.55	kJ/mol	Joback Method
hf	-836.79	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	76.75	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.402		Crippen Method
mcvol	271.730	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2283.00		NIST Webbook
rinpol	2283.00		NIST Webbook
tb	821.13	K	Joback Method
tc	1036.41	K	Joback Method
tf	458.73	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.80	J/mol×K	821.13	Joback Method
cpg	926.29	J/mol×K	857.01	Joback Method
cpg	945.10	J/mol×K	892.89	Joback Method
cpg	962.23	J/mol×K	928.77	Joback Method
cpg	977.73	J/mol×K	964.65	Joback Method
cpg	991.60	J/mol×K	1000.53	Joback Method
cpg	1003.86	J/mol×K	1036.41	Joback Method
dvisc	0.0012919	Pa×s	458.73	Joback Method

dvisc	0.0006292	Pa×s	519.13	Joback Method
dvisc	0.0003560	Pa×s	579.53	Joback Method
dvisc	0.0002243	Pa×s	639.93	Joback Method
dvisc	0.0001530	Pa×s	700.33	Joback Method
dvisc	0.0001109	Pa×s	760.73	Joback Method
dvisc	0.0000843	Pa×s	821.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339761&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