1,2-Cyclohexanedicarboxylic acid, decyl methyl ester

Inchi: InChI=1S/C19H34O4/c1-3-4-5-6-7-8-9-12-15-23-19(21)17-14-11-10-13-16(17)18(20)22-2

InchiKey: KFELCXUDOADCIU-UHFFFAOYSA-N

Formula: C19H34O4

SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-342.00	kJ/mol	Joback Method
hf	-891.11	kJ/mol	Joback Method
hfus	43.45	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.650		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	2289.00		NIST Webbook
rinpol	2289.00		NIST Webbook
tb	801.58	K	Joback Method
tc	996.17	K	Joback Method
tf	451.35	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.76	J/mol×K	801.58	Joback Method
cpg	927.91	J/mol×K	834.01	Joback Method
cpg	945.79	J/mol×K	866.44	Joback Method
cpg	962.41	J/mol×K	898.87	Joback Method
cpg	977.79	J/mol×K	931.31	Joback Method
cpg	991.95	J/mol×K	963.74	Joback Method
cpg	1004.88	J/mol×K	996.17	Joback Method
dvisc	0.0011198	Pa×s	451.35	Joback Method

dvisc	0.0005626	Pa×s	509.72	Joback Method
dvisc	0.0003257	Pa×s	568.09	Joback Method
dvisc	0.0002087	Pa×s	626.46	Joback Method
dvisc	0.0001443	Pa×s	684.84	Joback Method
dvisc	0.0001057	Pa×s	743.21	Joback Method
dvisc	0.0000810	Pa×s	801.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339657&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