cis-Cyclohex-4-en-1,2-dicarboxylic acid, isohexyl nonyl ester

Inchi: InChI=1S/C23H40O4/c1-4-5-6-7-8-9-12-17-26-22(24)20-15-10-11-16-21(20)23(25)27-18

InchiKey: DKICQLQCSBGJMM-UHFFFAOYSA-N

Formula: C23H40O4

SMILES: CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C

Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-280.80	kJ/mol	Joback Method
hf	-921.17	kJ/mol	Joback Method
hfus	51.50	kJ/mol	Joback Method
hvap	85.13	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.842		Crippen Method
mcvol	334.650	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		NIST Webbook
tb	891.82	K	Joback Method
tc	1094.61	K	Joback Method
tf	482.19	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.49	J/mol×K	891.82	Joback Method
cpg	1206.62	J/mol×K	1060.81	Joback Method
cpg	1193.46	J/mol×K	1027.01	Joback Method
cpg	1178.89	J/mol×K	993.22	Joback Method
cpg	1162.89	J/mol×K	959.42	Joback Method
cpg	1145.43	J/mol×K	925.62	Joback Method
cpg	1218.41	J/mol×K	1094.61	Joback Method
dvisc	0.0000458	Pa×s	891.82	Joback Method

dvisc	0.0000608	Pa×s	823.55	Joback Method
dvisc	0.0000847	Pa×s	755.28	Joback Method
dvisc	0.0001263	Pa×s	687.00	Joback Method
dvisc	0.0002055	Pa×s	618.73	Joback Method
dvisc	0.0003773	Pa×s	550.46	Joback Method
dvisc	0.0008228	Pa×s	482.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382685&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