cis-Cyclohex-4-en-1,2-dicarboxylic acid, hexyl 3-methylbutyl ester

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

InchiKey: YQFPEDBYLQODPK-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CCCCCCOC(=O)C1CC=CCC1C(=O)OCCC(C)C

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-314.48	kJ/mol	Joback Method
hf	-838.61	kJ/mol	Joback Method
hfus	41.14	kJ/mol	Joback Method
hvap	76.22	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.282		Crippen Method
mcvol	278.290	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	800.30	K	Joback Method
tc	997.70	K	Joback Method
tf	437.11	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.99	J/mol×K	800.30	Joback Method
cpg	962.35	J/mol×K	964.80	Joback Method
cpg	948.76	J/mol×K	931.90	Joback Method
cpg	933.94	J/mol×K	899.00	Joback Method
cpg	917.88	J/mol×K	866.10	Joback Method
cpg	900.57	J/mol×K	833.20	Joback Method
cpg	974.75	J/mol×K	997.70	Joback Method
dvisc	0.0000798	Pa×s	800.30	Joback Method

dvisc	0.0001047	Pa×s	739.77	Joback Method
dvisc	0.0001442	Pa×s	679.24	Joback Method
dvisc	0.0002113	Pa×s	618.71	Joback Method
dvisc	0.0003365	Pa×s	558.17	Joback Method
dvisc	0.0006002	Pa×s	497.64	Joback Method
dvisc	0.0012563	Pa×s	437.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382823&Units=SI

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