cis-Cyclohex-4-en-1,2-dicarboxylic acid, butyl undecyl ester

Inchi: InChI=1S/C23H40O4/c1-3-5-7-8-9-10-11-12-15-19-27-23(25)21-17-14-13-16-20(21)22(2
InchiKey: JLLCENQFWFQBLX-UHFFFAOYSA-N
Formula: C23H40O4
SMILES: CCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-278.36	kJ/mol	Joback Method
hf	-915.89	kJ/mol	Joback Method
hfus	55.03	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.986		Crippen Method
mcvol	334.650	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rinpol	2594.00		NIST Webbook
rinpol	2594.00		NIST Webbook
tb	892.26	K	Joback Method
tc	1094.33	K	Joback Method
tf	497.19	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.05	J/mol×K	892.26	Joback Method
cpg	1206.16	J/mol×K	1060.65	Joback Method
cpg	1192.96	J/mol×K	1026.97	Joback Method
cpg	1178.38	J/mol×K	993.30	Joback Method
cpg	1162.38	J/mol×K	959.62	Joback Method
cpg	1144.95	J/mol×K	925.94	Joback Method
cpg	1218.01	J/mol×K	1094.33	Joback Method
dvisc	0.0000502	Pa×s	892.26	Joback Method

dvisc	0.0000655	Pa×s	826.42	Joback Method
dvisc	0.0000897	Pa×s	760.57	Joback Method
dvisc	0.0001302	Pa×s	694.73	Joback Method
dvisc	0.0002044	Pa×s	628.88	Joback Method
dvisc	0.0003567	Pa×s	563.03	Joback Method
dvisc	0.0007213	Pa×s	497.19	Joback Method

Sources

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=U382753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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