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

Inchi: InChI=1S/C21H36O4/c1-3-5-6-7-8-9-10-11-14-17-25-21(23)19-16-13-12-15-18(19)20(22
InchiKey: METHQUDQVSRNCO-UHFFFAOYSA-N
Formula: C21H36O4
SMILES: CCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-295.20	kJ/mol	Joback Method
hf	-874.61	kJ/mol	Joback Method
hfus	49.85	kJ/mol	Joback Method
hvap	81.06	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.206		Crippen Method
mcvol	306.470	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2414.00		NIST Webbook
rinpol	2414.00		NIST Webbook
tb	846.50	K	Joback Method
tc	1043.73	K	Joback Method
tf	474.65	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.48	J/mol×K	846.50	Joback Method
cpg	1021.11	J/mol×K	879.37	Joback Method
cpg	1038.41	J/mol×K	912.24	Joback Method
cpg	1054.39	J/mol×K	945.12	Joback Method
cpg	1069.09	J/mol×K	977.99	Joback Method
cpg	1082.51	J/mol×K	1010.86	Joback Method
cpg	1094.68	J/mol×K	1043.73	Joback Method
dvisc	0.0008903	Pa×s	474.65	Joback Method

dvisc	0.0004499	Pa×s	536.62	Joback Method
dvisc	0.0002619	Pa×s	598.60	Joback Method
dvisc	0.0001687	Pa×s	660.58	Joback Method
dvisc	0.0001172	Pa×s	722.55	Joback Method
dvisc	0.0000862	Pa×s	784.52	Joback Method
dvisc	0.0000664	Pa×s	846.50	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=U382751&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