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

Inchi: InChI=1S/C22H38O4/c1-3-5-7-9-10-14-18-26-22(24)20-16-12-11-15-19(20)21(23)25-17-

InchiKey: YWWMZRLKRSAVIQ-UHFFFAOYSA-N

Formula: C22H38O4

SMILES: CCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCC

Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-286.78	kJ/mol	Joback Method
hf	-895.25	kJ/mol	Joback Method
hfus	52.44	kJ/mol	Joback Method
hvap	83.29	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.596		Crippen Method
mcvol	320.560	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
rinpol	2482.00		NIST Webbook
rinpol	2482.00		NIST Webbook
tb	869.38	K	Joback Method
tc	1068.63	K	Joback Method
tf	485.92	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.97	J/mol×K	869.38	Joback Method
cpg	1144.06	J/mol×K	1035.42	Joback Method
cpg	1130.74	J/mol×K	1002.21	Joback Method
cpg	1116.09	J/mol×K	969.01	Joback Method
cpg	1100.10	J/mol×K	935.80	Joback Method
cpg	1082.73	J/mol×K	902.59	Joback Method
cpg	1156.08	J/mol×K	1068.63	Joback Method
dvisc	0.0000578	Pa×s	869.38	Joback Method

dvisc	0.0000753	Pa×s	805.47	Joback Method
dvisc	0.0001027	Pa×s	741.56	Joback Method
dvisc	0.0001484	Pa×s	677.65	Joback Method
dvisc	0.0002318	Pa×s	613.74	Joback Method
dvisc	0.0004013	Pa×s	549.83	Joback Method
dvisc	0.0008030	Pa×s	485.92	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=U382665&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