cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(isohexyl) ester

Inchi: InChI=1S/C20H34O4/c1-15(2)9-7-13-23-19(21)17-11-5-6-12-18(17)20(22)24-14-8-10-16

InchiKey: PEVISEDIXJXZQL-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CC(C)CCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-308.50	kJ/mol	Joback Method
hf	-864.53	kJ/mol	Joback Method
hfus	40.21	kJ/mol	Joback Method
hvap	78.06	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.528		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
tb	822.74	K	Joback Method
tc	1022.27	K	Joback Method
tf	433.38	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.60	J/mol×K	822.74	Joback Method
cpg	961.44	J/mol×K	856.00	Joback Method
cpg	978.93	J/mol×K	889.25	Joback Method
cpg	995.09	J/mol×K	922.51	Joback Method
cpg	1009.94	J/mol×K	955.76	Joback Method
cpg	1023.50	J/mol×K	989.02	Joback Method
cpg	1035.78	J/mol×K	1022.27	Joback Method
dvisc	0.0013422	Pa×s	433.38	Joback Method

dvisc	0.0005809	Pa×s	498.27	Joback Method
dvisc	0.0003050	Pa×s	563.17	Joback Method
dvisc	0.0001829	Pa×s	628.06	Joback Method
dvisc	0.0001207	Pa×s	692.95	Joback Method
dvisc	0.0000855	Pa×s	757.85	Joback Method
dvisc	0.0000640	Pa×s	822.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382682&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

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