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

Inchi: InChI=1S/C20H34O4/c1-3-5-7-11-15-23-19(21)17-13-9-10-14-18(17)20(22)24-16-12-8-6

InchiKey: PTDFEHUSXWHNHR-UHFFFAOYSA-N

Formula: C20H34O4

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

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-303.62	kJ/mol	Joback Method
hf	-853.97	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	78.84	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.816		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	823.62	K	Joback Method
tc	1019.58	K	Joback Method
tf	463.38	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.63	J/mol×K	823.62	Joback Method
cpg	960.14	J/mol×K	856.28	Joback Method
cpg	977.37	J/mol×K	888.94	Joback Method
cpg	993.34	J/mol×K	921.60	Joback Method
cpg	1008.06	J/mol×K	954.26	Joback Method
cpg	1021.56	J/mol×K	986.92	Joback Method
cpg	1033.84	J/mol×K	1019.58	Joback Method
dvisc	0.0009829	Pa×s	463.38	Joback Method

dvisc	0.0005024	Pa×s	523.42	Joback Method
dvisc	0.0002948	Pa×s	583.46	Joback Method
dvisc	0.0001911	Pa×s	643.50	Joback Method
dvisc	0.0001334	Pa×s	703.54	Joback Method
dvisc	0.0000985	Pa×s	763.58	Joback Method
dvisc	0.0000761	Pa×s	823.62	Joback Method

Sources

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=U382664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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