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

Inchi: InChI=1S/C22H30O4/c1-2-3-4-10-16-25-21(23)19-13-8-9-14-20(19)22(24)26-17-15-18-1

InchiKey: VBPRPRSWYOEFPZ-UHFFFAOYSA-N

Formula: C22H30O4

SMILES: CCCCCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-174.37	kJ/mol	Joback Method
hf	-658.72	kJ/mol	Joback Method
hfus	46.48	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.478		Crippen Method
mcvol	296.800	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook
tb	896.06	K	Joback Method
tc	1113.65	K	Joback Method
tf	512.34	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.83	J/mol×K	896.06	Joback Method
cpg	984.41	J/mol×K	932.32	Joback Method
cpg	999.45	J/mol×K	968.59	Joback Method
cpg	1013.01	J/mol×K	1004.85	Joback Method
cpg	1025.10	J/mol×K	1041.12	Joback Method
cpg	1035.78	J/mol×K	1077.38	Joback Method
cpg	1045.08	J/mol×K	1113.65	Joback Method
dvisc	0.0006920	Pa×s	512.34	Joback Method

dvisc	0.0003666	Pa×s	576.29	Joback Method
dvisc	0.0002205	Pa×s	640.25	Joback Method
dvisc	0.0001455	Pa×s	704.20	Joback Method
dvisc	0.0001029	Pa×s	768.15	Joback Method
dvisc	0.0000767	Pa×s	832.11	Joback Method
dvisc	0.0000596	Pa×s	896.06	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=U382793&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