cis-Cyclohex-4-en-1,2-dicarboxylic acid, heptyl isohexyl ester

Inchi: InChI=1S/C21H36O4/c1-4-5-6-7-10-15-24-20(22)18-13-8-9-14-19(18)21(23)25-16-11-12

InchiKey: BHBIYJITKKOMFS-UHFFFAOYSA-N

Formula: C21H36O4

SMILES: CCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-297.64	kJ/mol	Joback Method
hf	-879.89	kJ/mol	Joback Method
hfus	46.32	kJ/mol	Joback Method
hvap	80.68	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.062		Crippen Method
mcvol	306.470	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
tb	846.06	K	Joback Method
tc	1044.69	K	Joback Method
tf	459.65	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.95	J/mol×K	846.06	Joback Method
cpg	1083.30	J/mol×K	1011.58	Joback Method
cpg	1069.87	J/mol×K	978.48	Joback Method
cpg	1055.15	J/mol×K	945.37	Joback Method
cpg	1039.10	J/mol×K	912.27	Joback Method
cpg	1021.70	J/mol×K	879.16	Joback Method
cpg	1095.45	J/mol×K	1044.69	Joback Method
dvisc	0.0000608	Pa×s	846.06	Joback Method

dvisc	0.0000802	Pa×s	781.66	Joback Method
dvisc	0.0001112	Pa×s	717.26	Joback Method
dvisc	0.0001644	Pa×s	652.86	Joback Method
dvisc	0.0002648	Pa×s	588.45	Joback Method
dvisc	0.0004795	Pa×s	524.05	Joback Method
dvisc	0.0010253	Pa×s	459.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382683&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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