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

Inchi: InChI=1S/C23H32O4/c1-2-3-4-5-11-17-26-22(24)20-14-9-10-15-21(20)23(25)27-18-16-1

InchiKey: ITJVMDIEDMSPCX-UHFFFAOYSA-N

Formula: C23H32O4

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

Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-165.95	kJ/mol	Joback Method
hf	-679.36	kJ/mol	Joback Method
hfus	49.07	kJ/mol	Joback Method
hvap	87.79	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.868		Crippen Method
mcvol	310.890	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2710.00		NIST Webbook
rinpol	2710.00		NIST Webbook
tb	918.94	K	Joback Method
tc	1136.69	K	Joback Method
tf	523.61	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.16	J/mol×K	918.94	Joback Method
cpg	1044.66	J/mol×K	955.23	Joback Method
cpg	1059.60	J/mol×K	991.52	Joback Method
cpg	1073.02	J/mol×K	1027.82	Joback Method
cpg	1084.95	J/mol×K	1064.11	Joback Method
cpg	1095.45	J/mol×K	1100.40	Joback Method
cpg	1104.55	J/mol×K	1136.69	Joback Method
dvisc	0.0006237	Pa×s	523.61	Joback Method

dvisc	0.0003268	Pa×s	589.50	Joback Method
dvisc	0.0001951	Pa×s	655.39	Joback Method
dvisc	0.0001279	Pa×s	721.28	Joback Method
dvisc	0.0000900	Pa×s	787.16	Joback Method
dvisc	0.0000669	Pa×s	853.05	Joback Method
dvisc	0.0000519	Pa×s	918.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382794&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