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

Inchi: InChI=1S/C21H28O4/c1-2-3-9-15-24-20(22)18-12-7-8-13-19(18)21(23)25-16-14-17-10-5

InchiKey: HSSYHHDKGGGDJV-UHFFFAOYSA-N

Formula: C21H28O4

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

Mol. weight [g/mol]: 344.44

Physical Properties

Property code	Value	Unit	Source
gf	-182.79	kJ/mol	Joback Method
hf	-638.08	kJ/mol	Joback Method
hfus	43.89	kJ/mol	Joback Method
hvap	83.34	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.088		Crippen Method
mcvol	282.710	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2508.00		NIST Webbook
rinpol	2508.00		NIST Webbook
tb	873.18	K	Joback Method
tc	1091.36	K	Joback Method
tf	501.07	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.07	J/mol×K	873.18	Joback Method
cpg	924.73	J/mol×K	909.54	Joback Method
cpg	939.87	J/mol×K	945.91	Joback Method
cpg	953.54	J/mol×K	982.27	Joback Method
cpg	965.78	J/mol×K	1018.63	Joback Method
cpg	976.61	J/mol×K	1054.99	Joback Method
cpg	986.08	J/mol×K	1091.36	Joback Method
dvisc	0.0007647	Pa×s	501.07	Joback Method

dvisc	0.0004098	Pa×s	563.09	Joback Method
dvisc	0.0002485	Pa×s	625.11	Joback Method
dvisc	0.0001649	Pa×s	687.12	Joback Method
dvisc	0.0001172	Pa×s	749.14	Joback Method
dvisc	0.0000877	Pa×s	811.16	Joback Method
dvisc	0.0000684	Pa×s	873.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382791&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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