

cis-Cyclohex-4-en-1,2-dicarboxylic acid, pentyl 3-phenylpropyl ester

Inchi:	InChI=1S/C22H30O4/c1-2-3-9-16-25-21(23)19-14-7-8-15-20(19)22(24)26-17-10-13-18-1
InchiKey:	LOKDAKKKIAGOBT-UHFFFAOYSA-N
Formula:	C22H30O4
SMILES:	CCCCCOC(=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
mvol	296.800	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2618.00		NIST Webbook
tb	896.06	K	Joback Method
tc	1113.65	K	Joback Method
tf	512.34	K	Joback Method
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.83	J/molxK	896.06	Joback Method
cpg	1035.78	J/molxK	1077.38	Joback Method
cpg	1025.10	J/molxK	1041.12	Joback Method
cpg	1013.01	J/molxK	1004.85	Joback Method
cpg	999.45	J/molxK	968.59	Joback Method
cpg	984.41	J/molxK	932.32	Joback Method
cpg	1045.08	J/molxK	1113.65	Joback Method
dvisc	0.0000596	Paxs	896.06	Joback Method
dvisc	0.0000767	Paxs	832.11	Joback Method

dvisc	0.0001029	Paxs	768.15	Joback Method
dvisc	0.0001455	Paxs	704.20	Joback Method
dvisc	0.0002205	Paxs	640.25	Joback Method
dvisc	0.0003666	Paxs	576.29	Joback Method
dvisc	0.0006920	Paxs	512.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U382775&Units=SI

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

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