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

Inchi: InChI=1S/C24H34O4/c1-2-3-4-5-11-18-27-23(25)21-16-9-10-17-22(21)24(26)28-19-12-1

InchiKey: RCVYSFMRNOETRG-UHFFFAOYSA-N

Formula: C24H34O4

SMILES: CCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 386.52

Physical Properties

Property code	Value	Unit	Source
gf	-157.53	kJ/mol	Joback Method
hf	-700.00	kJ/mol	Joback Method
hfus	51.66	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.258		Crippen Method
mcvol	324.980	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	941.82	K	Joback Method
tc	1160.54	K	Joback Method
tf	534.88	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.00	J/mol×K	941.82	Joback Method
cpg	1105.43	J/mol×K	978.27	Joback Method
cpg	1120.26	J/mol×K	1014.73	Joback Method
cpg	1133.53	J/mol×K	1051.18	Joback Method
cpg	1145.29	J/mol×K	1087.63	Joback Method
cpg	1155.59	J/mol×K	1124.09	Joback Method
cpg	1164.46	J/mol×K	1160.54	Joback Method
dvisc	0.0005599	Pa×s	534.88	Joback Method

dvisc	0.0002904	Pa×s	602.70	Joback Method
dvisc	0.0001720	Pa×s	670.53	Joback Method
dvisc	0.0001121	Pa×s	738.35	Joback Method
dvisc	0.0000786	Pa×s	806.17	Joback Method
dvisc	0.0000582	Pa×s	874.00	Joback Method
dvisc	0.0000450	Pa×s	941.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382778&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