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

Inchi: InChI=1S/C23H32O4/c1-18(2)10-8-16-26-22(24)20-14-6-7-15-21(20)23(25)27-17-9-13-1

InchiKey: QPLRVZQHNVUEPP-UHFFFAOYSA-N

Formula: C23H32O4

SMILES: CC(C)CCCOC(=O)C1CC=CCC1C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-168.39	kJ/mol	Joback Method
hf	-684.64	kJ/mol	Joback Method
hfus	45.55	kJ/mol	Joback Method
hvap	87.40	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.724		Crippen Method
mcvol	310.890	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	2678.00		NIST Webbook
rinpol	2678.00		NIST Webbook
tb	918.50	K	Joback Method
tc	1138.10	K	Joback Method
tf	508.61	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.61	J/mol×K	918.50	Joback Method
cpg	1045.22	J/mol×K	955.10	Joback Method
cpg	1060.22	J/mol×K	991.70	Joback Method
cpg	1073.66	J/mol×K	1028.30	Joback Method
cpg	1085.59	J/mol×K	1064.90	Joback Method
cpg	1096.04	J/mol×K	1101.50	Joback Method
cpg	1105.05	J/mol×K	1138.10	Joback Method
dvisc	0.0006968	Pa×s	508.61	Joback Method

dvisc	0.0003414	Pa×s	576.93	Joback Method
dvisc	0.0001945	Pa×s	645.24	Joback Method
dvisc	0.0001234	Pa×s	713.56	Joback Method
dvisc	0.0000848	Pa×s	781.87	Joback Method
dvisc	0.0000619	Pa×s	850.18	Joback Method
dvisc	0.0000473	Pa×s	918.50	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=U382776&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