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

Inchi: InChI=1S/C20H26O4/c1-15(2)14-24-20(22)18-11-7-6-10-17(18)19(21)23-13-12-16-8-4-3

InchiKey: KKNVKFIYBCSWKH-UHFFFAOYSA-N

Formula: C20H26O4

SMILES: CC(C)COC(=O)C1CC=CCC1C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-193.65	kJ/mol	Joback Method
hf	-622.72	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	80.73	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.554		Crippen Method
mcvol	268.620	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	849.86	K	Joback Method
tc	1072.21	K	Joback Method
tf	474.80	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.47	J/mol×K	849.86	Joback Method
cpg	866.39	J/mol×K	886.92	Joback Method
cpg	881.76	J/mol×K	923.98	Joback Method
cpg	895.63	J/mol×K	961.03	Joback Method
cpg	908.03	J/mol×K	998.09	Joback Method
cpg	919.00	J/mol×K	1035.15	Joback Method
cpg	928.55	J/mol×K	1072.21	Joback Method
dvisc	0.0009512	Pa×s	474.80	Joback Method

dvisc	0.0004811	Pa×s	537.31	Joback Method
dvisc	0.0002804	Pa×s	599.82	Joback Method
dvisc	0.0001810	Pa×s	662.33	Joback Method
dvisc	0.0001260	Pa×s	724.84	Joback Method
dvisc	0.0000929	Pa×s	787.35	Joback Method
dvisc	0.0000716	Pa×s	849.86	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=U382789&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