1,2-Cyclohexanedicarboxylic acid, 2-biphenyl ethyl ester

Inchi: InChI=1S/C22H24O4/c1-2-25-21(23)18-13-6-7-14-19(18)22(24)26-20-15-9-8-12-17(20)1

InchiKey: GMZVCHXNGJYGBY-UHFFFAOYSA-N

Formula: C22H24O4

SMILES: CCOC(=O)C1CCCCC1C(=O)Oc1ccccc1-c1ccccc1

Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-101.55	kJ/mol	Joback Method
hf	-491.44	kJ/mol	Joback Method
hfus	38.91	kJ/mol	Joback Method
hvap	88.21	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.628		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2605.00		NIST Webbook
rinpol	2605.00		NIST Webbook
tb	928.56	K	Joback Method
tc	1173.03	K	Joback Method
tf	550.52	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.91	J/mol×K	928.56	Joback Method
cpg	910.92	J/mol×K	969.31	Joback Method
cpg	924.09	J/mol×K	1010.05	Joback Method
cpg	935.47	J/mol×K	1050.80	Joback Method
cpg	945.11	J/mol×K	1091.54	Joback Method
cpg	953.06	J/mol×K	1132.29	Joback Method
cpg	959.38	J/mol×K	1173.03	Joback Method
dvisc	0.0005365	Pa×s	550.52	Joback Method

dvisc	0.0003060	Pa×s	613.53	Joback Method
dvisc	0.0001937	Pa×s	676.53	Joback Method
dvisc	0.0001326	Pa×s	739.54	Joback Method
dvisc	0.0000963	Pa×s	802.55	Joback Method
dvisc	0.0000733	Pa×s	865.55	Joback Method
dvisc	0.0000579	Pa×s	928.56	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=U339593&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