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

Inchi: InChI=1S/C24H28O4/c1-2-3-17-27-23(25)20-14-7-8-15-21(20)24(26)28-22-16-10-9-13-1

InchiKey: AVRHQIICPUNRRP-UHFFFAOYSA-N

Formula: C24H28O4

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

Mol. weight [g/mol]: 380.48

Physical Properties

Property code	Value	Unit	Source
gf	-84.71	kJ/mol	Joback Method
hf	-532.72	kJ/mol	Joback Method
hfus	44.09	kJ/mol	Joback Method
hvap	92.66	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.409		Crippen Method
mcvol	305.520	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	2778.00		NIST Webbook
rinpol	2778.00		NIST Webbook
tb	974.32	K	Joback Method
tc	1214.61	K	Joback Method
tf	573.06	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.67	J/mol×K	974.32	Joback Method
cpg	1029.18	J/mol×K	1014.37	Joback Method
cpg	1041.85	J/mol×K	1054.42	Joback Method
cpg	1052.74	J/mol×K	1094.47	Joback Method
cpg	1061.90	J/mol×K	1134.52	Joback Method
cpg	1069.40	J/mol×K	1174.56	Joback Method
cpg	1075.30	J/mol×K	1214.61	Joback Method
dvisc	0.0004358	Pa×s	573.06	Joback Method

dvisc	0.0002432	Pa×s	639.94	Joback Method
dvisc	0.0001515	Pa×s	706.81	Joback Method
dvisc	0.0001025	Pa×s	773.69	Joback Method
dvisc	0.0000738	Pa×s	840.57	Joback Method
dvisc	0.0000557	Pa×s	907.44	Joback Method
dvisc	0.0000437	Pa×s	974.32	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=U339594&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