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

Inchi: InChI=1S/C25H30O4/c1-2-3-11-18-28-24(26)21-15-7-8-16-22(21)25(27)29-23-17-10-9-1

InchiKey: VVKSMWGRGQRBCD-UHFFFAOYSA-N

Formula: C25H30O4

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

Mol. weight [g/mol]: 394.50

Physical Properties

Property code	Value	Unit	Source
gf	-76.29	kJ/mol	Joback Method
hf	-553.36	kJ/mol	Joback Method
hfus	46.68	kJ/mol	Joback Method
hvap	94.89	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.799		Crippen Method
mcvol	319.610	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	2871.00		NIST Webbook
tb	997.20	K	Joback Method
tc	1236.63	K	Joback Method
tf	584.33	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.72	J/mol×K	997.20	Joback Method
cpg	1088.98	J/mol×K	1037.11	Joback Method
cpg	1101.38	J/mol×K	1077.01	Joback Method
cpg	1112.00	J/mol×K	1116.92	Joback Method
cpg	1120.89	J/mol×K	1156.82	Joback Method
cpg	1128.13	J/mol×K	1196.73	Joback Method
cpg	1133.77	J/mol×K	1236.63	Joback Method
dvisc	0.0003907	Pa×s	584.33	Joback Method
dvisc	0.0002158	Pa×s	653.14	Joback Method

dvisc	0.0001334	Pa×s	721.95	Joback Method
dvisc	0.0000897	Pa×s	790.77	Joback Method
dvisc	0.0000643	Pa×s	859.58	Joback Method
dvisc	0.0000484	Pa×s	928.39	Joback Method
dvisc	0.0000379	Pa×s	997.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339595&Units=SI
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

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