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

Inchi: InChI=1S/C28H36O4/c1-2-3-4-5-6-14-21-31-27(29)24-18-10-11-19-25(24)28(30)32-26-2

InchiKey: NITKFZFCTSUEQP-UHFFFAOYSA-N

Formula: C28H36O4

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

Mol. weight [g/mol]: 436.58

Physical Properties

Property code	Value	Unit	Source
gf	-51.03	kJ/mol	Joback Method
hf	-615.28	kJ/mol	Joback Method
hfus	54.45	kJ/mol	Joback Method
hvap	101.57	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	6.969		Crippen Method
mcvol	361.880	ml/mol	McGowan Method
pc	1114.82	kPa	Joback Method
rinpol	3183.00		NIST Webbook
rinpol	3183.00		NIST Webbook
tb	1065.84	K	Joback Method
tc	1308.19	K	Joback Method
tf	618.14	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.96	J/mol×K	1065.84	Joback Method
cpg	1270.49	J/mol×K	1106.23	Joback Method
cpg	1282.09	J/mol×K	1146.62	Joback Method
cpg	1291.85	J/mol×K	1187.01	Joback Method
cpg	1299.83	J/mol×K	1227.41	Joback Method
cpg	1306.13	J/mol×K	1267.80	Joback Method
cpg	1310.81	J/mol×K	1308.19	Joback Method
dvisc	0.0002762	Pa×s	618.14	Joback Method

dvisc	0.0001481	Pa×s	692.76	Joback Method
dvisc	0.0000897	Pa×s	767.37	Joback Method
dvisc	0.0000593	Pa×s	841.99	Joback Method
dvisc	0.0000420	Pa×s	916.61	Joback Method
dvisc	0.0000313	Pa×s	991.22	Joback Method
dvisc	0.0000243	Pa×s	1065.84	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=U339599&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