Diethyl biphenyl-4,4'-dicarboxylate

Other names: Diethyl-4,4'-diphenyldicarboxylate
Diethyl biphenyl-4,4'-dicarboxylate
4,4'-Biphenyldicarboxylic acid diethyl ester
Inchi: InChI=1S/C18H18O4/c1-3-21-17(19)15-9-5-13(6-10-15)14-7-11-16(12-8-14)18(20)22-4-2
InchiKey: SYTZNHBXNLYWAK-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: CCOC(=O)c1ccc(-c2ccc(C(=O)OCC)cc2)cc1
Mol. weight [g/mol]: 298.34

Physical Properties

Property code	Value	Unit	Source
af	0.8002		Cheméo Relay (1.0)
hf	-594.17	kJ/mol	Cheméo Relay (1.0)
hfus	35.25	kJ/mol	Joback Method
hvap	109.48	kJ/mol	Cheméo Relay (1.0)
ie	8.59	eV	Cheméo Relay (1.0)
log10ws	-5.06		Cheméo Relay (1.0)
logp	3.707		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
tb	665.83	K	Cheméo Relay (1.0)
tc	877.55	K	Cheméo Relay (1.0)
tf	387.78	K	Cheméo Relay (1.0)
vc	0.860	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.96	J/mol×K	827.14	Joback Method
cpg	680.81	J/mol×K	865.36	Joback Method
cpg	693.42	J/mol×K	903.59	Joback Method
cpg	704.81	J/mol×K	941.81	Joback Method
cpg	715.01	J/mol×K	980.04	Joback Method
cpg	724.04	J/mol×K	1018.26	Joback Method

cpg	731.93	J/mol×K	1056.49	Joback Method
dvisc	0.0005404	Pa×s	514.82	Joback Method
dvisc	0.0003335	Pa×s	566.87	Joback Method
dvisc	0.0002232	Pa×s	618.93	Joback Method
dvisc	0.0001590	Pa×s	670.98	Joback Method
dvisc	0.0001189	Pa×s	723.03	Joback Method
dvisc	0.0000925	Pa×s	775.09	Joback Method
dvisc	0.0000743	Pa×s	827.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C47230386&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume