Methyl 3-(1,1'-biphenyl-4-yl)butanoate

Other names: 3-(4-Biphenylyl)butanoic acid methyl ester
Inchi: InChI=1S/C17H18O2/c1-13(12-17(18)19-2)14-8-10-16(11-9-14)15-6-4-3-5-7-15/h3-11,13
InchiKey: CRQARNDWPSBDKT-UHFFFAOYSA-N
Formula: C17H18O2
SMILES: COC(=O)CC(C)c1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 254.32
CAS: 24254-67-9

Physical Properties

Property code	Value	Unit	Source
gf	71.09	kJ/mol	Joback Method
hf	-182.70	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	67.42	kJ/mol	Joback Method
ie	8.00 ± 0.20	eV	NIST Webbook
log10ws	-4.96		Crippen Method
logp	4.020		Crippen Method
mcvol	210.310	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
tb	722.55	K	Joback Method
tc	956.32	K	Joback Method
tf	403.87	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.89	J/mol×K	722.55	Joback Method
cpg	642.70	J/mol×K	917.36	Joback Method
cpg	630.87	J/mol×K	878.40	Joback Method
cpg	617.93	J/mol×K	839.44	Joback Method
cpg	603.83	J/mol×K	800.47	Joback Method
cpg	588.49	J/mol×K	761.51	Joback Method
cpg	653.47	J/mol×K	956.32	Joback Method

dvisc	0.0001008	Pa×s	722.55	Joback Method
dvisc	0.0001302	Pa×s	669.44	Joback Method
dvisc	0.0001758	Pa×s	616.32	Joback Method
dvisc	0.0002512	Pa×s	563.21	Joback Method
dvisc	0.0003866	Pa×s	510.10	Joback Method
dvisc	0.0006579	Pa×s	456.98	Joback Method
dvisc	0.0012874	Pa×s	403.87	Joback Method

Sources

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=C24254679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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