3-Phenylpropionic acid, 4-biphenyl ester

Inchi: InChI=1S/C21H18O2/c22-21(16-11-17-7-3-1-4-8-17)23-20-14-12-19(13-15-20)18-9-5-2-6
InchiKey: MVWUPRQPAKZDTD-UHFFFAOYSA-N
Formula: C21H18O2
SMILES: O=C(CCc1ccccc1)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 302.37

Physical Properties

Property code	Value	Unit	Source
gf	219.62	kJ/mol	Joback Method
hf	-23.45	kJ/mol	Joback Method
hfus	34.67	kJ/mol	Joback Method
hvap	78.99	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	4.892		Crippen Method
mcvol	242.910	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	2777.00		NIST Webbook
rinpol	2777.00		NIST Webbook
tb	841.19	K	Joback Method
tc	1093.41	K	Joback Method
tf	490.37	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.99	J/mol×K	841.19	Joback Method
cpg	764.14	J/mol×K	1051.37	Joback Method
cpg	754.04	J/mol×K	1009.34	Joback Method
cpg	742.78	J/mol×K	967.30	Joback Method
cpg	730.25	J/mol×K	925.26	Joback Method
cpg	716.35	J/mol×K	883.23	Joback Method
cpg	773.17	J/mol×K	1093.41	Joback Method
dvisc	0.0000685	Pa×s	841.19	Joback Method

dvisc	0.0000871	Pa×s	782.72	Joback Method
dvisc	0.0001151	Pa×s	724.25	Joback Method
dvisc	0.0001598	Pa×s	665.78	Joback Method
dvisc	0.0002364	Pa×s	607.31	Joback Method
dvisc	0.0003799	Pa×s	548.84	Joback Method
dvisc	0.0006837	Pa×s	490.37	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=U354747&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