3-Phenylpropionic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C16H16O3/c1-18-14-8-10-15(11-9-14)19-16(17)12-7-13-5-3-2-4-6-13/h2-6,8-1

InchiKey: DLYKJMSERWHROY-UHFFFAOYSA-N

Formula: C16H16O3

SMILES: COc1ccc(OC(=O)CCc2ccccc2)cc1

Mol. weight [g/mol]: 256.30

Physical Properties

Property code	Value	Unit	Source
gf	-39.89	kJ/mol	Joback Method
hf	-289.00	kJ/mol	Joback Method
hfus	28.86	kJ/mol	Joback Method
hvap	67.99	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.233		Crippen Method
mcvol	202.090	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
tb	722.53	K	Joback Method
tc	953.08	K	Joback Method
tf	429.83	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.43	J/mol×K	722.53	Joback Method
cpg	559.93	J/mol×K	760.96	Joback Method
cpg	574.23	J/mol×K	799.38	Joback Method
cpg	587.37	J/mol×K	837.81	Joback Method
cpg	599.38	J/mol×K	876.23	Joback Method
cpg	610.29	J/mol×K	914.66	Joback Method
cpg	620.12	J/mol×K	953.08	Joback Method
dvisc	0.0008483	Pa×s	429.83	Joback Method

dvisc	0.0004890	Pa×s	478.61	Joback Method
dvisc	0.0003121	Pa×s	527.40	Joback Method
dvisc	0.0002150	Pa×s	576.18	Joback Method
dvisc	0.0001569	Pa×s	624.96	Joback Method
dvisc	0.0001199	Pa×s	673.75	Joback Method
dvisc	0.0000950	Pa×s	722.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307783&Units=SI

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