3-Phenylpropionic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C17H18O2/c1-13-10-14(2)12-16(11-13)19-17(18)9-8-15-6-4-3-5-7-15/h3-7,10-

InchiKey: CWKKOOCSSCRSTM-UHFFFAOYSA-N

Formula: C17H18O2

SMILES: Cc1cc(C)cc(OC(=O)CCc2ccccc2)c1

Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	63.90	kJ/mol	Joback Method
hf	-188.89	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.842		Crippen Method
mcvol	210.310	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	2006.00		NIST Webbook
rinpol	2006.00		NIST Webbook
tb	727.97	K	Joback Method
tc	958.19	K	Joback Method
tf	431.39	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.46	J/mol×K	727.97	Joback Method
cpg	586.59	J/mol×K	766.34	Joback Method
cpg	601.54	J/mol×K	804.71	Joback Method
cpg	615.34	J/mol×K	843.08	Joback Method
cpg	628.04	J/mol×K	881.45	Joback Method
cpg	639.67	J/mol×K	919.82	Joback Method
cpg	650.30	J/mol×K	958.19	Joback Method
dvisc	0.0009099	Pa×s	431.39	Joback Method

dvisc	0.0005331	Pa×s	480.82	Joback Method
dvisc	0.0003450	Pa×s	530.25	Joback Method
dvisc	0.0002405	Pa×s	579.68	Joback Method
dvisc	0.0001775	Pa×s	629.11	Joback Method
dvisc	0.0001369	Pa×s	678.54	Joback Method
dvisc	0.0001093	Pa×s	727.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307782&Units=SI
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

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