3-Phenylpropionic acid, 3-methylphenyl ester

Inchi: InChI=1S/C16H16O2/c1-13-6-5-9-15(12-13)18-16(17)11-10-14-7-3-2-4-8-14/h2-9,12H,10
InchiKey: BOGCCTWRSGWVMV-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: Cc1cccc(OC(=O)CCc2ccccc2)c1
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	65.11	kJ/mol	Joback Method
hf	-156.78	kJ/mol	Joback Method
hfus	27.68	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.533		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1922.00		NIST Webbook
rinpol	1922.00		NIST Webbook
tb	700.11	K	Joback Method
tc	933.89	K	Joback Method
tf	407.60	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.98	J/mol×K	700.11	Joback Method
cpg	533.95	J/mol×K	739.07	Joback Method
cpg	548.72	J/mol×K	778.04	Joback Method
cpg	562.33	J/mol×K	817.00	Joback Method
cpg	574.82	J/mol×K	855.96	Joback Method
cpg	586.26	J/mol×K	894.92	Joback Method
cpg	596.69	J/mol×K	933.89	Joback Method
dvisc	0.0011644	Pa×s	407.60	Joback Method

dvisc	0.0006540	Pa×s	456.35	Joback Method
dvisc	0.0004106	Pa×s	505.10	Joback Method
dvisc	0.0002798	Pa×s	553.86	Joback Method
dvisc	0.0002029	Pa×s	602.61	Joback Method
dvisc	0.0001544	Pa×s	651.36	Joback Method
dvisc	0.0001220	Pa×s	700.11	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=U307780&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