3-Phenylpropionic acid, phenyl ester

Inchi: InChI=1S/C15H14O2/c16-15(17-14-9-5-2-6-10-14)12-11-13-7-3-1-4-8-13/h1-10H,11-12H
InchiKey: VIGODTIMSIHKSD-UHFFFAOYSA-N
Formula: C15H14O2
SMILES: O=C(CCc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	66.32	kJ/mol	Joback Method
hf	-124.67	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	62.69	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.225		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1801.00		NIST Webbook
tb	672.25	K	Joback Method
tc	909.92	K	Joback Method
tf	383.81	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.75	J/mol×K	672.25	Joback Method
cpg	482.53	J/mol×K	711.86	Joback Method
cpg	497.08	J/mol×K	751.47	Joback Method
cpg	510.44	J/mol×K	791.09	Joback Method
cpg	522.68	J/mol×K	830.70	Joback Method
cpg	533.85	J/mol×K	870.31	Joback Method
cpg	544.01	J/mol×K	909.92	Joback Method
dvisc	0.0015219	Pa×s	383.81	Joback Method
dvisc	0.0008139	Pa×s	431.88	Joback Method

dvisc	0.0004934	Pa×s	479.96	Joback Method
dvisc	0.0003277	Pa×s	528.03	Joback Method
dvisc	0.0002330	Pa×s	576.10	Joback Method
dvisc	0.0001746	Pa×s	624.18	Joback Method
dvisc	0.0001364	Pa×s	672.25	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=U299021&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
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