3-Phenylpropionic acid, 3-ethylphenyl ester

Inchi: InChI=1S/C17H18O2/c1-2-14-9-6-10-16(13-14)19-17(18)12-11-15-7-4-3-5-8-15/h3-10,13
InchiKey: ORTPEEHZTWMQIU-UHFFFAOYSA-N
Formula: C17H18O2
SMILES: CCc1cccc(OC(=O)CCc2ccccc2)c1
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	73.53	kJ/mol	Joback Method
hf	-177.42	kJ/mol	Joback Method
hfus	30.27	kJ/mol	Joback Method
hvap	67.81	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.787		Crippen Method
mcvol	210.310	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	722.99	K	Joback Method
tc	952.42	K	Joback Method
tf	418.87	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.34	J/mol×K	722.99	Joback Method
cpg	587.63	J/mol×K	761.23	Joback Method
cpg	602.69	J/mol×K	799.47	Joback Method
cpg	616.59	J/mol×K	837.70	Joback Method
cpg	629.38	J/mol×K	875.94	Joback Method
cpg	641.10	J/mol×K	914.18	Joback Method
cpg	651.81	J/mol×K	952.42	Joback Method
dvisc	0.0010936	Pa×s	418.87	Joback Method

dvisc	0.0006053	Pa×s	469.56	Joback Method
dvisc	0.0003760	Pa×s	520.24	Joback Method
dvisc	0.0002542	Pa×s	570.93	Joback Method
dvisc	0.0001831	Pa×s	621.62	Joback Method
dvisc	0.0001386	Pa×s	672.30	Joback Method
dvisc	0.0001091	Pa×s	722.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354742&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

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