

3-Phenylpropionic acid, 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C17H18O2/c1-13-7-6-10-16(14(13)2)19-17(18)12-11-15-8-4-3-5-9-15/h3-10H,1
InchiKey:	URRUQWQULBEXIF-UHFFFAOYSA-N
Formula:	C17H18O2
SMILES:	Cc1cccc(OC(=O)CCc2ccccc2)c1C
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
rinsol	2131.00		NIST Webbook
tb	727.97	K	Joback Method
tc	958.19	K	Joback Method
tf	431.39	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.46	J/molxK	727.97	Joback Method
cpg	586.59	J/molxK	766.34	Joback Method
cpg	601.54	J/molxK	804.71	Joback Method
cpg	615.34	J/molxK	843.08	Joback Method
cpg	628.04	J/molxK	881.45	Joback Method
cpg	639.67	J/molxK	919.82	Joback Method
cpg	650.30	J/molxK	958.19	Joback Method
dvisc	0.0009099	Paxs	431.39	Joback Method
dvisc	0.0005331	Paxs	480.82	Joback Method

dvisc	0.0003450	Paxs	530.25	Joback Method
dvisc	0.0002405	Paxs	579.68	Joback Method
dvisc	0.0001775	Paxs	629.11	Joback Method
dvisc	0.0001369	Paxs	678.54	Joback Method
dvisc	0.0001093	Paxs	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=U354743&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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