Benzenepropanoic acid, 2,5-dimethoxy-

Other names:	3-(2,5-Dimethoxyphenyl)propionic acid
Inchi:	InChI=1S/C11H14O4/c1-14-9-4-5-10(15-2)8(7-9)3-6-11(12)13/h4-5,7H,3,6H2,1-2H3,(H,1
InchiKey:	JENQUCZZZGYHRW-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	COc1ccc(OC)c(CCC(=O)O)c1
Mol. weight [g/mol]:	210.23
CAS:	10538-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-340.85	kJ/mol	Joback Method
hf	-586.03	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	71.92	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.721		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	678.61	K	Joback Method
tc	875.09	K	Joback Method
tf	420.40	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.40	J/mol×K	678.61	Joback Method
cpg	433.78	J/mol×K	711.36	Joback Method
cpg	444.55	J/mol×K	744.10	Joback Method
cpg	454.68	J/mol×K	776.85	Joback Method
cpg	464.20	J/mol×K	809.60	Joback Method
cpg	473.08	J/mol×K	842.34	Joback Method
cpg	481.32	J/mol×K	875.09	Joback Method
dvisc	0.0009642	Pa×s	420.40	Joback Method

dvisc	0.0004463	Pa×s	463.44	Joback Method
dvisc	0.0002355	Pa×s	506.47	Joback Method
dvisc	0.0001373	Pa×s	549.50	Joback Method
dvisc	0.0000866	Pa×s	592.54	Joback Method
dvisc	0.0000582	Pa×s	635.58	Joback Method
dvisc	0.0000411	Pa×s	678.61	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=C10538495&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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