

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/molxK	678.61	Joback Method
cpg	433.78	J/molxK	711.36	Joback Method
cpg	444.55	J/molxK	744.10	Joback Method
cpg	454.68	J/molxK	776.85	Joback Method
cpg	464.20	J/molxK	809.60	Joback Method
cpg	473.08	J/molxK	842.34	Joback Method
cpg	481.32	J/molxK	875.09	Joback Method
dvisc	0.0009642	Paxs	420.40	Joback Method

dvisc	0.0004463	Paxs	463.44	Joback Method
dvisc	0.0002355	Paxs	506.47	Joback Method
dvisc	0.0001373	Paxs	549.50	Joback Method
dvisc	0.0000866	Paxs	592.54	Joback Method
dvisc	0.0000582	Paxs	635.58	Joback Method
dvisc	0.0000411	Paxs	678.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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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