3-(2,5-Dimethoxyphenyl)propionic acid

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

Physical Properties

Property code	Value	Unit	Source
hf	-622.28	kJ/mol	Cheméo Relay (1.0)
hfus	25.57	kJ/mol	Joback Method
ie	8.07	eV	Cheméo Relay (1.0)
log10ws	-2.17		Cheméo Relay (1.0)
logp	1.721		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
tb	596.43	K	Cheméo Relay (1.0)
tf	372.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.40	J/mol×K	678.61	Joback Method
cpg	481.32	J/mol×K	875.09	Joback Method
cpg	473.08	J/mol×K	842.34	Joback Method
cpg	464.20	J/mol×K	809.60	Joback Method
cpg	454.68	J/mol×K	776.85	Joback Method
cpg	444.55	J/mol×K	744.10	Joback Method
cpg	433.78	J/mol×K	711.36	Joback Method
dvisc	0.0001373	Pa×s	549.50	Joback Method
dvisc	0.0000411	Pa×s	678.61	Joback Method
dvisc	0.0000582	Pa×s	635.58	Joback Method
dvisc	0.0000866	Pa×s	592.54	Joback Method
dvisc	0.0009642	Pa×s	420.40	Joback Method
dvisc	0.0002355	Pa×s	506.47	Joback Method

dvisc	0.0004463	Pa×s	463.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10538495&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point