3,5-Dimethoxyphenethylamine

Other names:	Benzeneethanamine, 3,5-dimethoxy-
Inchi:	InChI=1S/C10H15NO2/c1-12-9-5-8(3-4-11)6-10(7-9)13-2/h5-7H,3-4,11H2,1-2H3
InchiKey:	ZHSFEDDRTVLPHH-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	COc1cc(CCN)cc(OC)c1
Mol. weight [g/mol]:	181.23
CAS:	3213-28-3

Physical Properties

Property code	Value	Unit	Source
gf	-17.08	kJ/mol	Joback Method
hf	-266.79	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	56.92	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.205		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	582.21	K	Joback Method
tc	795.30	K	Joback Method
tf	381.64	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.65	J/mol×K	582.21	Joback Method
cpg	378.45	J/mol×K	617.72	Joback Method
cpg	391.58	J/mol×K	653.24	Joback Method
cpg	404.04	J/mol×K	688.75	Joback Method
cpg	415.81	J/mol×K	724.27	Joback Method
cpg	426.90	J/mol×K	759.78	Joback Method
cpg	437.30	J/mol×K	795.30	Joback Method

Sources

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=C3213283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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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