2-(3,4-Dimethoxyphenyl)-2-methoxy-N,N-dimethyl

Inchi: InChI=1S/C13H21NO3/c1-14(2)9-13(17-5)10-6-7-11(15-3)12(8-10)16-4/h6-8,13H,9H2,1-
InchiKey: JDECRXOMHIGGFQ-UHFFFAOYSA-N
Formula: C13H21NO3
SMILES: COc1ccc(C(CN(C)C)OC)cc1OC
Mol. weight [g/mol]: 239.31

Physical Properties

Property code	Value	Unit	Source
gf	-54.93	kJ/mol	Joback Method
hf	-432.47	kJ/mol	Joback Method
hfus	25.75	kJ/mol	Joback Method
hvap	57.02	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.953		Crippen Method
mcvol	197.860	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1679.10		NIST Webbook
tb	612.74	K	Joback Method
tc	808.05	K	Joback Method
tf	371.89	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.79	J/mol×K	612.74	Joback Method
cpg	529.53	J/mol×K	645.29	Joback Method
cpg	545.47	J/mol×K	677.84	Joback Method
cpg	560.60	J/mol×K	710.40	Joback Method
cpg	574.93	J/mol×K	742.95	Joback Method
cpg	588.44	J/mol×K	775.50	Joback Method
cpg	601.14	J/mol×K	808.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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