Propanamide, N-(2,5-dimethoxyphenyl)-2,2-dimethyl-

Inchi: InChI=1S/C13H19NO3/c1-13(2,3)12(15)14-10-8-9(16-4)6-7-11(10)17-5/h6-8H,1-5H3,(H,
InchiKey: ZDMQBPDGIJATFQ-UHFFFAOYSA-N
Formula: C13H19NO3
SMILES: COc1ccc(OC)c(NC(=O)C(C)(C)C)c1
Mol. weight [g/mol]: 237.29

Physical Properties

Property code	Value	Unit	Source
gf	-94.96	kJ/mol	Joback Method
hf	-430.36	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.688		Crippen Method
mcvol	193.560	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	679.13	K	Joback Method
tc	892.68	K	Joback Method
tf	437.20	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.34	J/mol×K	679.13	Joback Method
cpg	540.60	J/mol×K	714.72	Joback Method
cpg	554.89	J/mol×K	750.31	Joback Method
cpg	568.23	J/mol×K	785.90	Joback Method
cpg	580.64	J/mol×K	821.49	Joback Method
cpg	592.16	J/mol×K	857.09	Joback Method
cpg	602.80	J/mol×K	892.68	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307199&Units=SI

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