2-Butenamide, N-(2,5-dimethoxyphenyl)-3-methyl-

Inchi: InChI=1S/C13H17NO3/c1-9(2)7-13(15)14-11-8-10(16-3)5-6-12(11)17-4/h5-8H,1-4H3,(H,
InchiKey: SIOULVGQXKBFSI-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: COc1ccc(OC)c(NC(=O)C=C(C)C)c1
Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-26.13	kJ/mol	Joback Method
hf	-314.18	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.608		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	686.40	K	Joback Method
tc	900.12	K	Joback Method
tf	415.74	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.47	J/mol×K	686.40	Joback Method
cpg	513.86	J/mol×K	722.02	Joback Method
cpg	527.38	J/mol×K	757.64	Joback Method
cpg	540.04	J/mol×K	793.26	Joback Method
cpg	551.87	J/mol×K	828.88	Joback Method
cpg	562.86	J/mol×K	864.50	Joback Method
cpg	573.05	J/mol×K	900.12	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=U307272&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