Butanamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C12H17NO3/c1-4-5-12(14)13-10-8-9(15-2)6-7-11(10)16-3/h6-8H,4-5H2,1-3H3
InchiKey: VBJWZQLKFYYTHQ-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: CCCC(=O)Nc1cc(OC)ccc1OC
Mol. weight [g/mol]: 223.27

Physical Properties

Property code	Value	Unit	Source
gf	-106.22	kJ/mol	Joback Method
hf	-400.97	kJ/mol	Joback Method
hfus	29.17	kJ/mol	Joback Method
hvap	63.91	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.442		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	1854.00		NIST Webbook
tb	659.48	K	Joback Method
tc	865.30	K	Joback Method
tf	423.51	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.58	J/mol×K	659.48	Joback Method
cpg	484.80	J/mol×K	693.78	Joback Method
cpg	498.23	J/mol×K	728.09	Joback Method
cpg	510.88	J/mol×K	762.39	Joback Method
cpg	522.73	J/mol×K	796.69	Joback Method
cpg	533.79	J/mol×K	830.99	Joback Method
cpg	544.05	J/mol×K	865.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306917&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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