Acetamide, N-(2,5-dimethoxyphenyl)-2-phenyl-

Inchi: InChI=1S/C16H17NO3/c1-19-13-8-9-15(20-2)14(11-13)17-16(18)10-12-6-4-3-5-7-12/h3-9
InchiKey: ZREUHORSMKPNIE-UHFFFAOYSA-N
Formula: C16H17NO3
SMILES: COc1ccc(OC)c(NC(=O)Cc2ccccc2)c1
Mol. weight [g/mol]: 271.31

Physical Properties

Property code	Value	Unit	Source
gf	39.87	kJ/mol	Joback Method
hf	-247.00	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	75.09	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.885		Crippen Method
mcvol	212.070	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	2322.00		NIST Webbook
rinpol	2322.00		NIST Webbook
tb	777.68	K	Joback Method
tc	1007.26	K	Joback Method
tf	495.01	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.77	J/mol×K	777.68	Joback Method
cpg	611.22	J/mol×K	815.94	Joback Method
cpg	624.49	J/mol×K	854.21	Joback Method
cpg	636.58	J/mol×K	892.47	Joback Method
cpg	647.54	J/mol×K	930.73	Joback Method
cpg	657.39	J/mol×K	969.00	Joback Method
cpg	666.14	J/mol×K	1007.26	Joback Method

Sources

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=U307146&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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