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

Inchi: InChI=1S/C16H17NO3S/c1-19-12-8-9-15(20-2)14(10-12)17-16(18)11-21-13-6-4-3-5-7-13

InchiKey: DQTUHVGJPPLSIT-UHFFFAOYSA-N

Formula: C16H17NO3S

SMILES: COc1ccc(OC)c(NC(=O)CSc2ccccc2)c1

Mol. weight [g/mol]: 303.38

Physical Properties

Property code	Value	Unit	Source
gf	72.99	kJ/mol	Joback Method
hf	-205.13	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	81.91	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.435		Crippen Method
mcvol	228.420	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	846.46	K	Joback Method
tc	1089.44	K	Joback Method
tf	529.41	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.81	J/mol×K	846.46	Joback Method
cpg	661.90	J/mol×K	886.96	Joback Method
cpg	673.61	J/mol×K	927.45	Joback Method
cpg	683.94	J/mol×K	967.95	Joback Method
cpg	692.91	J/mol×K	1008.45	Joback Method
cpg	700.55	J/mol×K	1048.95	Joback Method
cpg	706.87	J/mol×K	1089.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307210&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