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

Inchi: InChI=1S/C16H25NO3/c1-4-5-6-7-8-9-16(18)17-14-12-13(19-2)10-11-15(14)20-3/h10-12
InchiKey: VRBOQYRNOHMGJE-UHFFFAOYSA-N
Formula: C16H25NO3
SMILES: CCCCCCCC(=O)Nc1cc(OC)ccc1OC
Mol. weight [g/mol]: 279.37

Physical Properties

Property code	Value	Unit	Source
gf	-72.54	kJ/mol	Joback Method
hf	-483.53	kJ/mol	Joback Method
hfus	39.53	kJ/mol	Joback Method
hvap	72.81	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.003		Crippen Method
mcvol	235.830	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook
tb	751.00	K	Joback Method
tc	948.50	K	Joback Method
tf	468.59	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.95	J/mol×K	751.00	Joback Method
cpg	701.87	J/mol×K	783.92	Joback Method
cpg	716.83	J/mol×K	816.83	Joback Method
cpg	730.85	J/mol×K	849.75	Joback Method
cpg	743.93	J/mol×K	882.66	Joback Method
cpg	756.08	J/mol×K	915.58	Joback Method
cpg	767.32	J/mol×K	948.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306928&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

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