Pentanamide, N-(2,5-dimethoxyphenyl)-5-chloro-

Inchi: InChI=1S/C13H18ClNO3/c1-17-10-6-7-12(18-2)11(9-10)15-13(16)5-3-4-8-14/h6-7,9H,3-5

InchiKey: RUIMICHAILIILK-UHFFFAOYSA-N

Formula: C13H18ClNO3

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

Mol. weight [g/mol]: 271.74

Physical Properties

Property code	Value	Unit	Source
gf	-109.73	kJ/mol	Joback Method
hf	-437.35	kJ/mol	Joback Method
hfus	35.96	kJ/mol	Joback Method
hvap	70.52	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.051		Crippen Method
mcvol	205.800	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	2228.00		NIST Webbook
tb	719.79	K	Joback Method
tc	926.41	K	Joback Method
tf	464.70	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.34	J/mol×K	719.79	Joback Method
cpg	563.10	J/mol×K	754.23	Joback Method
cpg	576.00	J/mol×K	788.66	Joback Method
cpg	588.05	J/mol×K	823.10	Joback Method
cpg	599.24	J/mol×K	857.54	Joback Method
cpg	609.58	J/mol×K	891.97	Joback Method
cpg	619.08	J/mol×K	926.41	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=U307363&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