Propanamide, N-(2,5-dimethoxyphenyl)-3-chloro-

Inchi: InChI=1S/C11H14ClNO3/c1-15-8-3-4-10(16-2)9(7-8)13-11(14)5-6-12/h3-4,7H,5-6H2,1-2
InchiKey: QLZAYTWEEVKOOY-UHFFFAOYSA-N
Formula: C11H14ClNO3
SMILES: COc1ccc(OC)c(NC(=O)CCCl)c1
Mol. weight [g/mol]: 243.69

Physical Properties

Property code	Value	Unit	Source
gf	-126.57	kJ/mol	Joback Method
hf	-396.07	kJ/mol	Joback Method
hfus	30.78	kJ/mol	Joback Method
hvap	66.07	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.271		Crippen Method
mcvol	177.620	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
tb	674.03	K	Joback Method
tc	886.36	K	Joback Method
tf	442.16	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.61	J/mol×K	674.03	Joback Method
cpg	458.31	J/mol×K	709.42	Joback Method
cpg	470.25	J/mol×K	744.81	Joback Method
cpg	481.42	J/mol×K	780.19	Joback Method
cpg	491.81	J/mol×K	815.58	Joback Method
cpg	501.42	J/mol×K	850.97	Joback Method
cpg	510.26	J/mol×K	886.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307230&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