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

Inchi: InChI=1S/C11H14ClNO3/c1-7(12)11(14)13-9-6-8(15-2)4-5-10(9)16-3/h4-7H,1-3H3,(H,13

InchiKey: RMRDVDAALOHFAM-UHFFFAOYSA-N

Formula: C11H14ClNO3

SMILES: COc1ccc(OC)c(NC(=O)C(C)Cl)c1

Mol. weight [g/mol]: 243.69

Physical Properties

Property code	Value	Unit	Source
gf	-129.01	kJ/mol	Joback Method
hf	-401.35	kJ/mol	Joback Method
hfus	27.26	kJ/mol	Joback Method
hvap	65.68	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.270		Crippen Method
mcvol	177.620	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
tb	673.59	K	Joback Method
tc	889.90	K	Joback Method
tf	427.16	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.14	J/mol×K	673.59	Joback Method
cpg	459.12	J/mol×K	709.64	Joback Method
cpg	471.29	J/mol×K	745.69	Joback Method
cpg	482.64	J/mol×K	781.74	Joback Method
cpg	493.18	J/mol×K	817.80	Joback Method
cpg	502.90	J/mol×K	853.85	Joback Method
cpg	511.81	J/mol×K	889.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307488&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