Urea, 1-(2-chloroethyl)-3-(3,4,5-trimethoxyphenyl)-

Inchi: InChI=1S/C12H17ClN2O4/c1-17-9-6-8(15-12(16)14-5-4-13)7-10(18-2)11(9)19-3/h6-7H,4

InchiKey: RVSXAKGVAATORR-UHFFFAOYSA-N

Formula: C12H17ClN2O4

SMILES: COc1cc(NC(=O)NCCCl)cc(OC)c1OC

Mol. weight [g/mol]: 288.73

CAS: 33021-68-0

Physical Properties

Property code	Value	Unit	Source
gf	-143.39	kJ/mol	Joback Method
hf	-506.93	kJ/mol	Joback Method
hfus	39.27	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.073		Crippen Method
mcvol	207.560	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
tb	774.48	K	Joback Method
tc	983.34	K	Joback Method
tf	540.84	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.31	J/mol×K	774.48	Joback Method
cpg	585.74	J/mol×K	809.29	Joback Method
cpg	597.26	J/mol×K	844.10	Joback Method
cpg	607.86	J/mol×K	878.91	Joback Method
cpg	617.52	J/mol×K	913.72	Joback Method
cpg	626.23	J/mol×K	948.53	Joback Method
cpg	633.98	J/mol×K	983.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33021680&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume