Acetamide, N-(2,5-dimethoxyphenyl)-2,2,2-trichloro-

Inchi: InChI=1S/C10H10Cl3NO3/c1-16-6-3-4-8(17-2)7(5-6)14-9(15)10(11,12)13/h3-5H,1-2H3,(

InchiKey: MXINBMRGIGQXDX-UHFFFAOYSA-N

Formula: C10H10Cl3NO3

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

Mol. weight [g/mol]: 298.55

Physical Properties

Property code	Value	Unit	Source
gf	-156.01	kJ/mol	Joback Method
hf	-415.66	kJ/mol	Joback Method
hfus	29.17	kJ/mol	Joback Method
hvap	71.31	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.012		Crippen Method
mcvol	188.010	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1975.00		NIST Webbook
tb	722.78	K	Joback Method
tc	956.63	K	Joback Method
tf	493.15	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.03	J/mol×K	722.78	Joback Method
cpg	454.41	J/mol×K	761.75	Joback Method
cpg	463.92	J/mol×K	800.73	Joback Method
cpg	472.58	J/mol×K	839.70	Joback Method
cpg	480.42	J/mol×K	878.68	Joback Method
cpg	487.45	J/mol×K	917.65	Joback Method
cpg	493.72	J/mol×K	956.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307220&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