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

Inchi: InChI=1S/C10H10F3NO3/c1-16-6-3-4-8(17-2)7(5-6)14-9(15)10(11,12)13/h3-5H,1-2H3,(H

InchiKey: ICQKZCPTDWBKRC-UHFFFAOYSA-N

Formula: C10H10F3NO3

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

Mol. weight [g/mol]: 249.19

Physical Properties

Property code	Value	Unit	Source
gf	-704.65	kJ/mol	Joback Method
hf	-956.77	kJ/mol	Joback Method
hfus	25.82	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.205		Crippen Method
mcvol	156.600	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1446.00		NIST Webbook
tb	608.30	K	Joback Method
tc	804.16	K	Joback Method
tf	405.16	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.07	J/mol×K	608.30	Joback Method
cpg	410.71	J/mol×K	640.94	Joback Method
cpg	421.66	J/mol×K	673.59	Joback Method
cpg	431.93	J/mol×K	706.23	Joback Method
cpg	441.54	J/mol×K	738.88	Joback Method
cpg	450.51	J/mol×K	771.52	Joback Method
cpg	458.84	J/mol×K	804.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307313&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