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

Inchi: InChI=1S/C11H10F5NO3/c1-19-6-3-4-8(20-2)7(5-6)17-9(18)10(12,13)11(14,15)16/h3-5H

InchiKey: AZCAFCWWFSJUCD-UHFFFAOYSA-N

Formula: C11H10F5NO3

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

Mol. weight [g/mol]: 299.19

Physical Properties

Property code	Value	Unit	Source
gf	-1083.01	kJ/mol	Joback Method
hf	-1378.38	kJ/mol	Joback Method
hfus	27.16	kJ/mol	Joback Method
hvap	55.00	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.840		Crippen Method
mcvol	174.230	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1444.00		NIST Webbook
rinpol	1444.00		NIST Webbook
tb	626.49	K	Joback Method
tc	813.83	K	Joback Method
tf	420.03	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.26	J/mol×K	626.49	Joback Method
cpg	478.95	J/mol×K	657.71	Joback Method
cpg	489.88	J/mol×K	688.94	Joback Method
cpg	500.08	J/mol×K	720.16	Joback Method
cpg	509.57	J/mol×K	751.38	Joback Method
cpg	518.38	J/mol×K	782.61	Joback Method
cpg	526.55	J/mol×K	813.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307334&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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