Butanamide, N-(2,5-dimethoxyphenyl)-2,2,3,3,4,4,4-heptafluoro

Inchi: InChI=1S/C12H10F7NO3/c1-22-6-3-4-8(23-2)7(5-6)20-9(21)10(13,14)11(15,16)12(17,18

InchiKey: QKDMKFZROUUMBQ-UHFFFAOYSA-N

Formula: C12H10F7NO3

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

Mol. weight [g/mol]: 349.20

Physical Properties

Property code	Value	Unit	Source
gf	-1461.37	kJ/mol	Joback Method
hf	-1799.99	kJ/mol	Joback Method
hfus	28.49	kJ/mol	Joback Method
hvap	54.30	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.475		Crippen Method
mcvol	191.860	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1476.00		NIST Webbook
tb	644.68	K	Joback Method
tc	824.93	K	Joback Method
tf	434.90	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.34	J/mol×K	644.68	Joback Method
cpg	547.97	J/mol×K	674.72	Joback Method
cpg	558.80	J/mol×K	704.76	Joback Method
cpg	568.85	J/mol×K	734.80	Joback Method
cpg	578.17	J/mol×K	764.84	Joback Method
cpg	586.81	J/mol×K	794.89	Joback Method
cpg	594.79	J/mol×K	824.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307280&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