Benzamide, N-(2,5-dimethoxyphenyl)-2,3,4,5,6-pentafluoro-

Inchi: InChI=1S/C15H10F5NO3/c1-23-6-3-4-8(24-2)7(5-6)21-15(22)9-10(16)12(18)14(20)13(19

InchiKey: KEGIDEUTQPXEAB-UHFFFAOYSA-N

Formula: C15H10F5NO3

SMILES: COc1ccc(OC)c(NC(=O)c2c(F)c(F)c(F)c(F)c2F)c1

Mol. weight [g/mol]: 347.24

Physical Properties

Property code	Value	Unit	Source
gf	-990.75	kJ/mol	Joback Method
hf	-1264.26	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	72.09	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.652		Crippen Method
mcvol	206.830	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook
tb	776.05	K	Joback Method
tc	974.99	K	Joback Method
tf	549.29	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.76	J/mol×K	776.05	Joback Method
cpg	585.73	J/mol×K	809.21	Joback Method
cpg	595.91	J/mol×K	842.36	Joback Method
cpg	605.28	J/mol×K	875.52	Joback Method
cpg	613.83	J/mol×K	908.68	Joback Method
cpg	621.56	J/mol×K	941.84	Joback Method
cpg	628.47	J/mol×K	974.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307380&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