Benzamide, N-(2,5-dimethoxyphenyl)-4-nitro-

Inchi: InChI=1S/C15H14N2O5/c1-21-12-7-8-14(22-2)13(9-12)16-15(18)10-3-5-11(6-4-10)17(19
InchiKey: HUMYECVYADBLCY-UHFFFAOYSA-N
Formula: C15H14N2O5
SMILES: COc1ccc(OC)c(NC(=O)c2ccc([N+](=O)[O-])cc2)c1
Mol. weight [g/mol]: 302.28

Physical Properties

Property code	Value	Unit	Source
gf	57.37	kJ/mol	Joback Method
hf	-248.59	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	90.11	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	2.864		Crippen Method
mcvol	215.400	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	2712.00		NIST Webbook
rinpol	2712.00		NIST Webbook
tb	911.62	K	Joback Method
tc	1162.50	K	Joback Method
tf	639.87	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.53	J/mol×K	911.62	Joback Method
cpg	646.03	J/mol×K	953.43	Joback Method
cpg	655.20	J/mol×K	995.25	Joback Method
cpg	663.06	J/mol×K	1037.06	Joback Method
cpg	669.63	J/mol×K	1078.87	Joback Method
cpg	674.94	J/mol×K	1120.69	Joback Method
cpg	679.01	J/mol×K	1162.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307354&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