

Benzamide, 3-methoxy-N-(3-methoxybenzoyl)-N-ethyl-

Inchi: InChI=1S/C18H19NO4/c1-4-19(17(20)13-7-5-9-15(11-13)22-2)18(21)14-8-6-10-16(12-14)
InchiKey: COFLLHPMYFFSBQ-UHFFFAOYSA-N
Formula: C18H19NO4
SMILES: CCN(C(=O)c1cccc(OC)c1)C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 313.35

Physical Properties

Property code	Value	Unit	Source
gf	-50.82	kJ/mol	Joback Method
hf	-386.80	kJ/mol	Joback Method
hfus	38.27	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.006		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	2393.00		NIST Webbook
rinpol	2393.00		NIST Webbook
tb	839.58	K	Joback Method
tc	1066.51	K	Joback Method
tf	547.29	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.72	J/mol×K	839.58	Joback Method
cpg	721.53	J/mol×K	877.40	Joback Method
cpg	734.10	J/mol×K	915.22	Joback Method
cpg	745.44	J/mol×K	953.04	Joback Method
cpg	755.62	J/mol×K	990.87	Joback Method
cpg	764.65	J/mol×K	1028.69	Joback Method
cpg	772.58	J/mol×K	1066.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407522&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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