

Benzamide, N-[[4-[2-(dimethylamino)ethoxy]phenyl]methyl]-3,

Other names:	Trimethobenzamide N-[p-[2-(Dimethylamino)ethoxy]benzyl]-3,4,5-trimethoxybenzamide
Inchi:	InChI=1S/C21H28N2O5/c1-23(2)10-11-28-17-8-6-15(7-9-17)14-22-21(24)16-12-18(25-3)
InchiKey:	FEZBIKUBAYAZIU-UHFFFAOYSA-N
Formula:	C21H28N2O5
SMILES:	COc1cc(C(=O)NCc2ccc(OCCN(C)C)cc2)cc(OC)c1OC
Mol. weight [g/mol]:	388.46
CAS:	138-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-36.51	kJ/mol	Joback Method
hf	-570.05	kJ/mol	Joback Method
hfus	51.14	kJ/mol	Joback Method
hvap	94.41	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	2.583		Crippen Method
mcvol	304.240	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpola	3287.00		NIST Webbook
rinpola	3287.00		NIST Webbook
tb	959.32	K	Joback Method
tc	1181.30	K	Joback Method
tf	653.33	K	Joback Method
vc	1.127	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.12	J/molxK	959.32	Joback Method
cpg	990.24	J/molxK	996.32	Joback Method
cpg	1001.78	J/molxK	1033.31	Joback Method
cpg	1011.72	J/molxK	1070.31	Joback Method
cpg	1020.08	J/molxK	1107.31	Joback Method

cpg	1026.85	J/mol×K	1144.31	Joback Method
cpg	1032.04	J/mol×K	1181.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C138567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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