m-Terephthalanisidide

Other names:	3,3'-Dimethoxy terephthalanilide
	3',3''-3,3'-Dimethoxy terephthalanilide
	N,N'-Bis-(m-methoxyphenyl)terphtalamide
Inchi:	InChI=1S/C22H20N2O4/c1-27-19-7-3-5-17(13-19)23-21(25)15-9-11-16(12-10-15)22(26)2
InchiKey:	BTEAFZRBSOWUOB-UHFFFAOYSA-N
Formula:	C22H20N2O4
SMILES:	COc1cccc(NC(=O)c2ccc(C(=O)Nc3cccc(OC)c3)cc2)c1
Mol. weight [g/mol]:	376.41
CAS:	6957-81-9

Physical Properties

Property code	Value	Unit	Source
chs	-10966.30 ± 3.00	kJ/mol	NIST Webbook
gf	153.64	kJ/mol	Joback Method
hf	-340.00 ± 8.80	kJ/mol	NIST Webbook
hfs	-549.20 ± 3.20	kJ/mol	NIST Webbook
hfus	49.46	kJ/mol	Joback Method
hsub	209.00 ± 8.40	kJ/mol	NIST Webbook
hvap	104.56	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.208		Crippen Method
mcvol	284.400	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
tb	1050.66	K	Joback Method
tc	1302.73	K	Joback Method
tf	704.16	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.15	J/mol×K	1260.72	Joback Method
cpg	891.42	J/mol×K	1050.66	Joback Method
cpg	900.44	J/mol×K	1092.67	Joback Method

cpg	907.96	J/mol×K	1134.68	Joback Method
cpg	914.04	J/mol×K	1176.70	Joback Method
cpg	918.75	J/mol×K	1218.71	Joback Method
cpg	924.31	J/mol×K	1302.73	Joback Method
cps	458.10	J/mol×K	298.15	NIST Webbook
hsubt	209.20 ± 8.40	kJ/mol	190.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6957819&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume