

N,N'-Bis(o-methoxyphenyl)terephthalamide

Inchi:	InChI=1S/C22H20N2O4/c1-27-19-9-5-3-7-17(19)23-21(25)15-11-13-16(14-12-15)22(26)2
InchiKey:	JRZCFDYNUTXOCW-UHFFFAOYSA-N
Formula:	C22H20N2O4
SMILES:	COc1ccccc1NC(=O)c1ccc(C(=O)Nc2ccccc2OC)cc1
Mol. weight [g/mol]:	376.41
CAS:	36360-34-6

Physical Properties

Property code	Value	Unit	Source
chs	-11007.60 ± 3.40	kJ/mol	NIST Webbook
gf	153.64	kJ/mol	Joback Method
hf	-310.00 ± 5.40	kJ/mol	NIST Webbook
hfs	-507.90 ± 3.60	kJ/mol	NIST Webbook
hfus	49.46	kJ/mol	Joback Method
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	918.75	J/molxK	1218.71	Joback Method
cpg	922.15	J/molxK	1260.72	Joback Method
cpg	891.42	J/molxK	1050.66	Joback Method
cpg	900.44	J/molxK	1092.67	Joback Method
cpg	907.96	J/molxK	1134.68	Joback Method
cpg	914.04	J/molxK	1176.70	Joback Method
cpg	924.31	J/molxK	1302.73	Joback Method

hsubt	197.00 ± 4.20	kJ/mol	456.30	NIST Webbook
hsubt	197.50 ± 4.20	kJ/mol	190.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36360346&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
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

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