

Meso-2,3-dimethoxy-2,3-diphenylsuccinonitrile

Inchi:	InChI=1S/C18H16N2O2/c1-21-17(13-19,15-9-5-3-6-10-15)18(14-20,22-2)16-11-7-4-8-12
InchiKey:	IESMRPVAAQUHSX-HDICACEKSA-N
Formula:	C18H16N2O2
SMILES:	COC(C#N)(c1ccccc1)C(C#N)(OC)c1ccccc1
Mol. weight [g/mol]:	292.33
CAS:	61502-56-5

Physical Properties

Property code	Value	Unit	Source
chs	-9393.20 ± 1.90	kJ/mol	NIST Webbook
gf	387.54	kJ/mol	Joback Method
hf	170.00	kJ/mol	NIST Webbook
hfs	23.40 ± 1.90	kJ/mol	NIST Webbook
hfus	21.02	kJ/mol	Joback Method
hvap	83.40	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.117		Crippen Method
mcvol	231.460	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
tb	907.14	K	Joback Method
tc	1166.29	K	Joback Method
tf	524.74	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.74	J/molxK	907.14	Joback Method
cpg	692.09	J/molxK	950.33	Joback Method
cpg	702.36	J/molxK	993.52	Joback Method
cpg	711.67	J/molxK	1036.71	Joback Method
cpg	720.16	J/molxK	1079.91	Joback Method
cpg	727.96	J/molxK	1123.10	Joback Method
cpg	735.20	J/molxK	1166.29	Joback Method

Sources

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=C61502565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
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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