

m-Nitrobenzilidene-2-naphthylacetonitrile

Inchi:	InChI=1S/C19H12N2O2/c20-13-18(10-14-4-3-7-19(11-14)21(22)23)17-9-8-15-5-1-2-6-16
InchiKey:	NZTJYHFIPNUREJ-ZDLGFXPLSA-N
Formula:	C19H12N2O2
SMILES:	N#CC(=Cc1cccc([N+](=O)[O-])c1)c1ccc2ccccc2c1
Mol. weight [g/mol]:	300.31
CAS:	29476-43-5

Physical Properties

Property code	Value	Unit	Source
chs	-9423.75	kJ/mol	NIST Webbook
gf	661.71	kJ/mol	Joback Method
hf	467.25	kJ/mol	Joback Method
hfs	232.50	kJ/mol	NIST Webbook
hfus	41.05	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	4.812		Crippen Method
mcvol	226.090	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
tb	974.38	K	Joback Method
tc	1256.23	K	Joback Method
tf	604.03	K	Joback Method
vc	0.894	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.12	J/molxK	974.38	Joback Method
cpg	662.68	J/molxK	1021.36	Joback Method
cpg	673.78	J/molxK	1068.33	Joback Method
cpg	684.64	J/molxK	1115.31	Joback Method
cpg	695.47	J/molxK	1162.28	Joback Method
cpg	706.51	J/molxK	1209.26	Joback Method
cpg	717.98	J/molxK	1256.23	Joback Method

Sources

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=C29476435&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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