

o-Nitrobenzylidene-2,5-dimethylphenylacetone nitrile

Inchi: InChI=1S/C17H14N2O2/c1-12-7-8-13(2)16(9-12)15(11-18)10-14-5-3-4-6-17(14)19(20)21
InchiKey: SUCPQQDDIXAJJR-XNTDXEJSSA-N
Formula: C17H14N2O2
SMILES: Cc1ccc(C)c(C(C#N)=Cc2ccccc2[N+](=O)[O-])c1
Mol. weight [g/mol]: 278.31
CAS: 113366-20-4

Physical Properties

Property code	Value	Unit	Source
chs	-8840.00	kJ/mol	NIST Webbook
gf	528.59	kJ/mol	Joback Method
hf	305.99	kJ/mol	Joback Method
hfs	146.00	kJ/mol	NIST Webbook
hfus	38.46	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.276		Crippen Method
mcvol	217.370	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
tb	914.62	K	Joback Method
tc	1182.06	K	Joback Method
tf	561.31	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.33	J/molxK	914.62	Joback Method
cpg	632.10	J/molxK	959.19	Joback Method
cpg	642.94	J/molxK	1003.77	Joback Method
cpg	652.98	J/molxK	1048.34	Joback Method
cpg	662.34	J/molxK	1092.91	Joback Method
cpg	671.13	J/molxK	1137.49	Joback Method
cpg	679.48	J/molxK	1182.06	Joback Method

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=C113366204&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
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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