

(o-Nitrobenzylidene)phenylacetonitrile

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C15H10N2O2/c16-11-14(12-6-2-1-3-7-12)10-13-8-4-5-9-15(13)17(18)19/h1-10

QKDHOOPLFPJKV-GXDHUFHOSA-N

C15H10N2O2

N#CC(=Cc1ccccc1[N+](=O)[O-])c1ccccc1

250.25

19016-67-2

Physical Properties

Property code	Value	Unit	Source
chs	-7519.00	kJ/mol	NIST Webbook
chs	-7515.64	kJ/mol	NIST Webbook
gf	531.01	kJ/mol	Joback Method
hf	370.21	kJ/mol	Joback Method
hfs	187.00	kJ/mol	NIST Webbook
hfs	183.80	kJ/mol	NIST Webbook
hfus	34.06	kJ/mol	Joback Method
hvap	81.30	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.659		Crippen Method
mcvol	189.190	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	858.90	K	Joback Method
tc	1137.09	K	Joback Method
tf	513.73	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.14	J/mol×K	858.90	Joback Method
cpg	525.21	J/mol×K	905.26	Joback Method
cpg	535.30	J/mol×K	951.63	Joback Method
cpg	544.57	J/mol×K	997.99	Joback Method
cpg	553.19	J/mol×K	1044.36	Joback Method

cpg	561.29	J/mol×K	1090.72	Joback Method
cpg	569.03	J/mol×K	1137.09	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=C19016672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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