

Benzenamine, n-[(2-nitrophenyl)methylene]-

Other names:	Aniline, N-(o-nitrobenzylidene)- N-(o-Nitrobenzylidene)aniline N-(2-nitrobenzylidene)aniline
Inchi:	InChI=1S/C13H10N2O2/c16-15(17)13-9-5-4-6-11(13)10-14-12-7-2-1-3-8-12/h1-10H
InchiKey:	BBAZSPGQKPGVIJ-UHFFFAOYSA-N
Formula:	C13H10N2O2
SMILES:	O=[N+][O-]c1cccc1C=Nc1cccc1
Mol. weight [g/mol]:	226.24

Physical Properties

Property code	Value	Unit	Source
hf	245.01	kJ/mol	Cheméo Relay (1.0)
hvap	88.21	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-4.09		Cheméo Relay (1.0)
logp	3.345		Crippen Method
mcvol	169.610	ml/mol	McGowan Method
tb	620.13	K	Cheméo Relay (1.0)
tf	351.74	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17064776&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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