

Anthracene, 9-(2-nitroethenyl)-

Other names:	Anthracene, 9-(2-nitrovinyl)- 9-(2-Nitrovinyl)anthracene 9-(«omega»-Nitrovinyl)anthracene
Inchi:	InChI=1S/C16H11NO2/c18-17(19)10-9-16-14-7-3-1-5-12(14)11-13-6-2-4-8-15(13)16/h1-
InchiKey:	GYOMWYPUMGJROJ-MDZDMXLPSA-N
Formula:	C16H11NO2
SMILES:	O=[N+](O-)C=Cc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	249.26
CAS:	58349-77-2

Physical Properties

Property code	Value	Unit	Source
gf	506.06	kJ/mol	Joback Method
hf	328.62	kJ/mol	Joback Method
hfus	36.06	kJ/mol	Joback Method
hvap	74.64	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	4.240		Crippen Method
mcvol	186.740	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	796.08	K	Joback Method
tc	1068.36	K	Joback Method
tf	525.47	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.58	J/molxK	796.08	Joback Method
cpg	515.28	J/molxK	841.46	Joback Method
cpg	527.11	J/molxK	886.84	Joback Method
cpg	538.29	J/molxK	932.22	Joback Method
cpg	549.04	J/molxK	977.60	Joback Method
cpg	559.58	J/molxK	1022.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C58349772&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
mccvol:	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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