Acenaphthylene, 1,2-dihydro-5-nitro-

Other names:	Acenaphthene, 5-nitro-
	5-Nitroacenaphthene
	5-Nitroacenapthene
	NCI-C01967
	1,2-Dihydro-5-nitro-acenaphthylene
	5-Nan
	5-Nitronaphthalene ethylene
Inchi:	InChI=1S/C12H9NO2/c14-13(15)11-7-6-9-5-4-8-2-1-3-10(11)12(8)9/h1-3,6-7H,4-5H2
InchiKey:	CUARLQDWYSRQDF-UHFFFAOYSA-N
Formula:	C12H9NO2
SMILES:	O=[N+]([O-])c1ccc2c3c(cccc13)CC2
Mol. weight [g/mol]:	199.21
CAS:	602-87-9

Physical Properties

Property code	Value	Unit	Source
gf	356.44	kJ/mol	Joback Method
hf	190.72	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	64.85	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	2.847		Crippen Method
mcvol	143.280	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	337.65		NIST Webbook
rinpol	337.65		NIST Webbook
rinpol	337.45		NIST Webbook
tb	693.54	K	Joback Method
tc	959.27	K	Joback Method
tf	490.99	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.23	J/mol×K	693.54	Joback Method
cpg	381.05	J/mol×K	737.83	Joback Method
cpg	391.92	J/mol×K	782.12	Joback Method
cpg	402.01	J/mol×K	826.41	Joback Method
cpg	411.52	J/mol×K	870.69	Joback Method
cpg	420.60	J/mol×K	914.98	Joback Method
cpg	429.44	J/mol×K	959.27	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=C602879&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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