Anthracene, 9-nitro-

Other names: 5-Nitroanthracene
9-nitroanthracene
Inchi: InChI=1S/C14H9NO2/c16-15(17)14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9H
InchiKey: LSIKFJXEYJIZNB-UHFFFAOYSA-N
Formula: C14H9NO2
SMILES: O=[N+]([O-])c1c2ccccc2cc2ccccc12
Mol. weight [g/mol]: 223.23
CAS: 602-60-8

Physical Properties

Property code	Value	Unit	Source
ea	1.43 ± 0.10	eV	NIST Webbook
ea	1.77 ± 0.05	eV	NIST Webbook
gf	409.00	kJ/mol	Joback Method
hf	252.68	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hsub	115.40 ± 0.60	kJ/mol	NIST Webbook
hvap	70.23	kJ/mol	Joback Method
ie	7.88 ± 0.03	eV	NIST Webbook
ie	7.86 ± 0.01	eV	NIST Webbook
log10ws	-5.73		Crippen Method
logp	3.901		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	356.50		NIST Webbook
rinpol	357.42		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	365.70		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	356.50		NIST Webbook
rinpol	356.69		NIST Webbook
rinpol	356.62		NIST Webbook
rinpol	356.59		NIST Webbook
rinpol	357.11		NIST Webbook
rinpol	356.95		NIST Webbook
rinpol	357.42		NIST Webbook
rinpol	356.62		NIST Webbook

rinpol	357.42		NIST Webbook
tb	746.16	K	Joback Method
tc	1021.21	K	Joback Method
tf	508.01	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.68	J/mol×K	837.84	Joback Method
cpg	436.51	J/mol×K	792.00	Joback Method
cpg	485.75	J/mol×K	1021.21	Joback Method
cpg	476.86	J/mol×K	975.37	Joback Method
cpg	467.67	J/mol×K	929.53	Joback Method
cpg	458.00	J/mol×K	883.68	Joback Method
cpg	424.33	J/mol×K	746.16	Joback Method
hfust	20.10	kJ/mol	420.40	NIST Webbook
hsubt	111.90 ± 0.60	kJ/mol	369.00	NIST Webbook
psub	6.40e-04	kPa	373.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	3.54e-04	kPa	367.09	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	3.39e-04	kPa	367.09	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	4.31e-04	kPa	369.04	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	4.39e-04	kPa	369.04	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	4.27e-04	kPa	369.04	Thermochemistry of nitronaphthalenes and nitroanthracenes

psub	5.32e-04	kPa	371.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	5.26e-04	kPa	371.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	5.34e-04	kPa	371.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	3.42e-04	kPa	367.09	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	6.43e-04	kPa	373.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	6.47e-04	kPa	373.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	7.72e-04	kPa	375.00	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	7.73e-04	kPa	375.00	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	7.61e-04	kPa	375.00	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	9.28e-04	kPa	377.06	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	9.28e-04	kPa	377.06	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	9.24e-04	kPa	377.06	Thermochemistry of nitronaphthalenes and nitroanthracenes

psub	2.94e-04	kPa	365.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.91e-04	kPa	365.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.91e-04	kPa	365.26	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.38e-04	kPa	363.08	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.36e-04	kPa	363.08	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.36e-04	kPa	363.08	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.95e-04	kPa	361.11	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.96e-04	kPa	361.11	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.90e-04	kPa	361.11	Thermochemistry of nitronaphthalenes and nitroanthracenes

Sources

Thermochemistry of nitronaphthalenes and nitroanthracenes:	https://www.doi.org/10.1016/j.jct.2005.08.007
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=C602608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume