

9-Anthracenecarbonitrile

Other names:	9-Anthronitrile 9-Cyanoanthracene Anthracene-9-carbonitrile
Inchi:	InChI=1S/C15H9N/c16-10-15-13-7-3-1-5-11(13)9-12-6-2-4-8-14(12)15/h1-9H
InchiKey:	KEQZHLAEKAVZLY-UHFFFAOYSA-N
Formula:	C15H9N
SMILES:	N#Cc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	203.24
CAS:	1210-12-4

Physical Properties

Property code	Value	Unit	Source
ea	1.27 ± 0.10	eV	NIST Webbook
gf	515.05	kJ/mol	Joback Method
hf	407.68	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Joback Method
ie	7.80 ± 0.03	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-5.43		Crippen Method
logp	3.865		Crippen Method
mcvol	160.910	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	357.10		NIST Webbook
rinpol	350.70		NIST Webbook
tb	719.28	K	Joback Method
tc	979.82	K	Joback Method
tf	440.66	K	Joback Method
vc	0.637	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.10	J/mol×K	936.40	Joback Method

cpg	400.37	J/mol×K	719.28	Joback Method
cpg	412.09	J/mol×K	762.70	Joback Method
cpg	422.88	J/mol×K	806.13	Joback Method
cpg	432.88	J/mol×K	849.55	Joback Method
cpg	442.24	J/mol×K	892.97	Joback Method
cpg	459.62	J/mol×K	979.82	Joback Method
hfust	25.19	kJ/mol	445.20	NIST Webbook

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=C1210124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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
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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