

Anthraquinone, 2-amino-

Other names:	9,10-Anthracenedione, 2-amino- «beta»-Aminoanthraquinone 2-Amino-9,10-anthraquinone 2-Aminoanthraquinone AAQ NCI-C01876 2-Amino-9,10-anthracenedione 2-AAQ «beta»-Anthraquinonylamine beta-Aminoanthraquinone NSC 5
Inchi:	InChI=1S/C14H9NO2/c15-8-5-6-11-12(7-8)14(17)10-4-2-1-3-9(10)13(11)16/h1-7H,15H2
InchiKey:	XOGPDSATLSAZEK-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	<chem>Nc1ccc2c(c1)C(=O)c1cccc1C2=O</chem>
Mol. weight [g/mol]:	223.23
CAS:	117-79-3

Physical Properties

Property code	Value	Unit	Source
gf	164.76	kJ/mol	Joback Method
hf	-35.95	kJ/mol	Joback Method
hfus	22.31	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.044		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	407.06		NIST Webbook
rinpol	406.00		NIST Webbook
rinpol	406.03		NIST Webbook
rinpol	408.00		NIST Webbook
rinpol	406.00		NIST Webbook
tb	803.33	K	Joback Method
tc	1081.85	K	Joback Method
tf	524.00 ± 1.00	K	NIST Webbook
vc	0.613	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.33	J/mol×K	803.33	Joback Method
cpg	468.05	J/mol×K	849.75	Joback Method
cpg	479.54	J/mol×K	896.17	Joback Method
cpg	489.82	J/mol×K	942.59	Joback Method
cpg	498.96	J/mol×K	989.01	Joback Method
cpg	506.99	J/mol×K	1035.43	Joback Method
cpg	513.96	J/mol×K	1081.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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