

9,10-Anthracenedione, 1-amino-2,4-dibromo-

Other names:	Anthraquinone, 1-amino-2,4-dibromo- 1-Amino-2,4-dibromoanthraquinone 2,4-Dibromo-1-anthraquinonylamine NCI-C55458 1-Amino-2,4-dibromanthrachinon 1-Amino-2,4-dibromoanthra-9,10-quinone 1-Amino-2,4-dibromo-9,10-anthraquinone NSC 3529
Inchi:	InChI=1S/C14H7Br2NO2/c15-8-5-9(16)12(17)11-10(8)13(18)6-3-1-2-4-7(6)14(11)19/h1-5
InchiKey:	ZINRVIQBCHAZMM-UHFFFAOYSA-N
Formula:	C14H7Br2NO2
SMILES:	Nc1c(Br)cc(Br)c2c1C(=O)c1cccc1C2=O
Mol. weight [g/mol]:	381.02
CAS:	81-49-2

Physical Properties

Property code	Value	Unit	Source
gf	174.14	kJ/mol	Joback Method
hf	-6.23	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	86.67	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	3.569		Crippen Method
mcvol	197.860	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	945.61	K	Joback Method
tc	1240.65	K	Joback Method
tf	727.98	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.91	J/mol×K	945.61	Joback Method

cpg	512.11	J/mol×K	994.78	Joback Method
cpg	520.29	J/mol×K	1043.96	Joback Method
cpg	527.53	J/mol×K	1093.13	Joback Method
cpg	533.88	J/mol×K	1142.30	Joback Method
cpg	539.43	J/mol×K	1191.47	Joback Method
cpg	544.23	J/mol×K	1240.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81492&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
mcvol:	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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