

9,10-Anthracenedione, 2-methyl-1-nitro-

Other names:	Anthraquinone, 2-methyl-1-nitro- 1-Nitro-2-methylanthraquinone 2-Methyl-1-nitroanthraquinone NCI-C01923 1-N-2-Ma 2-Methyl-1-nitro-9,10-anthracenedione
Inchi:	InChI=1S/C15H9NO4/c1-8-6-7-11-12(13(8)16(19)20)15(18)10-5-3-2-4-9(10)14(11)17/h2
InchiKey:	FYXKXZFTZBYYNP-UHFFFAOYSA-N
Formula:	C15H9NO4
SMILES:	<chem>Cc1ccc2c(c1[N+](=O)[O-])C(=O)c1cccc1C2=O</chem>
Mol. weight [g/mol]:	267.24
CAS:	129-15-7

Physical Properties

Property code	Value	Unit	Source
gf	132.65	kJ/mol	Joback Method
hf	-112.61	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	81.32	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	2.679		Crippen Method
mcvol	184.390	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	910.50	K	Joback Method
tc	1194.00	K	Joback Method
tf	667.48	K	Joback Method
vc	0.722	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.97	J/mol×K	910.50	Joback Method
cpg	551.02	J/mol×K	957.75	Joback Method
cpg	560.74	J/mol×K	1005.00	Joback Method

cpg	569.17	J/mol×K	1052.25	Joback Method
cpg	576.36	J/mol×K	1099.50	Joback Method
cpg	582.35	J/mol×K	1146.75	Joback Method
cpg	587.19	J/mol×K	1194.00	Joback Method

Sources

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=C129157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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