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

Other names:	1-Amino-2-methyl-9,10-anthraquinone
	1-amino-2-methyl-9,10-anthracenedione
	1-amino-2-methylanthraquinone
	2-methyl-1-anthraquinonylamine
	C.I. 60700
	C.I. disperse orange 11
	C.I. solvent orange 35
	NCI-C01901
	NSC 39943
	NSC 667744
	Oranz disperzni 11
	acetate fast orange R
	acetoquinone light orange JL
	anthraquinone, 1-amino-2-methyl-
	artisil orange 3RP
	celliton orange R
	cilla orange R
	disperse orange
	disperse orange (anthraquinone dye)
	disperse orange 11
	duranol orange G
	microsetile orange RA
	nyloquinone orange JR
	perliton orange 3R
	serisol orange YL
	solvent orange 35
	supracet orange R
Inchi:	InChI=1S/C15H11NO2/c1-8-6-7-11-12(13(8)16)15(18)10-5-3-2-4-9(10)14(11)17/h2-7H,1
InchiKey:	ZLCUIOWQYBYEBG-UHFFFAOYSA-N
Formula:	C15H11NO2
SMILES:	Cc1ccc2c(c1N)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	237.25
CAS:	82-28-0

Physical Properties

Property code	Value	Unit	Source

gf	163.55	kJ/mol	Joback Method
hf	-68.06	kJ/mol	Joback Method
hfus	24.51	kJ/mol	Joback Method
hvap	75.37	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.353		Crippen Method
mcvol	176.950	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	831.19	K	Joback Method
tc	1103.62	K	Joback Method
tf	607.13	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.30	J/mol×K	831.19	Joback Method
cpg	520.33	J/mol×K	876.59	Joback Method
cpg	532.10	J/mol×K	922.00	Joback Method
cpg	542.66	J/mol×K	967.40	Joback Method
cpg	552.04	J/mol×K	1012.81	Joback Method
cpg	560.27	J/mol×K	1058.21	Joback Method
cpg	567.39	J/mol×K	1103.62	Joback Method
hsubt	124.60 ± 7.30	kJ/mol	374.00	NIST Webbook

Sources

Measurement of binary diffusion coefficient and solubility estimation for dyes in supercritical carbon dioxide by CIR method:	https://www.doi.org/10.1016/j.fluid.2016.01.010
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=C82280&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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