9,10-ANTHRACENEDIONE, 2-METHYL-

Other names:	Anthraquinone, 2-methyl-
	«beta»-Methylanthraquinone
	Techtoquinone
	Tectochinon
	Tectoquinone
	2-Methylanthraquinone
	2-Methylanthra-9,10-quinone
	NSC 607
	2-Methylanthracenedione
Inchi:	InChI=1S/C15H10O2/c1-9-6-7-12-13(8-9)15(17)11-5-3-2-4-10(11)14(12)16/h2-8H,1H3
InchiKey:	NJWGQARXZDRHCD-UHFFFAOYSA-N
Formula:	C15H10O2
SMILES:	Cc1ccc2c(c1)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	222.24

Physical Properties

Property code	Value	Unit	Source
af	0.6176		Cheméo Relay (1.0)
gf	106.73	kJ/mol	Joback Method
hf	-126.57	kJ/mol	Cheméo Relay (1.0)
hfus	19.71	kJ/mol	Joback Method
hvap	97.72	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-5.14		Cheméo Relay (1.0)
logp	2.770		Crippen Method
mcvol	166.970	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	2035.00		NIST Webbook
rinpol	352.70		NIST Webbook
rinpol	350.10		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2035.00		NIST Webbook
tb	650.95	K	Cheméo Relay (1.0)
tc	942.07	K	Cheméo Relay (1.0)
tf	449.17 ± 0.35	K	NIST Webbook
tf	449.45 ± 0.25	K	NIST Webbook
vc	0.625	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.00	J/mol×K	753.68	Joback Method
cpg	466.44	J/mol×K	798.53	Joback Method
cpg	479.63	J/mol×K	843.38	Joback Method
cpg	491.63	J/mol×K	888.23	Joback Method
cpg	502.47	J/mol×K	933.09	Joback Method
cpg	512.19	J/mol×K	977.94	Joback Method
cpg	520.84	J/mol×K	1022.79	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C84548&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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

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