

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:	<chem>Cc1ccc2c(c1)C(=O)c1cccc1C2=O</chem>
Mol. weight [g/mol]:	222.24
CAS:	84-54-8

Physical Properties

Property code	Value	Unit	Source
gf	106.73	kJ/mol	Joback Method
hf	-90.38	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	64.07	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	2.770		Crippen Method
mcvol	166.970	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	2035.00		NIST Webbook
rinpol	350.10		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2035.00		NIST Webbook
rinpol	352.70		NIST Webbook
tb	753.68	K	Joback Method
tc	1022.79	K	Joback Method
tf	449.17 ± 0.35	K	NIST Webbook
tf	449.45 ± 0.25	K	NIST Webbook
vc	0.639	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84548&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

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

vc: Critical Volume

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