

Benz(a)anthracene-7,12-dione

Other names:	Benzanthracene-7,12-dione Benzanthraquinone Benz[a]anthra-7,12-quinone Benz[a]anthracene-7,12-quinone C.I. 59000 Sirius Yellow G 1,2-Benzanthraquinone 1,2-Benzo-9,10-anthraquinone 1,2-Benzoanthraquinone NSC 7961 Benzo[a]anthracene-7,12-dione Benza(a)anthraquinone 7,12-Benz[a]anthracenequinone Benz[a]anthraquinone Benz[a]anthraquinone-7,12
Inchi:	InChI=1S/C18H10O2/c19-17-13-7-3-4-8-14(13)18(20)16-12-6-2-1-5-11(12)9-10-15(16)17
InchiKey:	LHMRXAIRPKSGDE-UHFFFAOYSA-N
Formula:	C18H10O2
SMILES:	O=C1c2ccccc2C(=O)c2c1ccc1cccc21
Mol. weight [g/mol]:	258.27
CAS:	2498-66-0

Physical Properties

Property code	Value	Unit	Source
chs	-8279.83	kJ/mol	NIST Webbook
gf	238.64	kJ/mol	Joback Method
hf	38.77	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hsub	82.80	kJ/mol	NIST Webbook
hvap	72.38	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.615		Crippen Method
mcvol	189.780	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	416.80		NIST Webbook
rinpol	417.46		NIST Webbook
rinpol	417.90		NIST Webbook

rmpol	416.46		NIST Webbook
rmpol	416.80		NIST Webbook
rmpol	2479.00		NIST Webbook
rmpol	2479.00		NIST Webbook
rmpol	417.26		NIST Webbook
rmpol	417.89		NIST Webbook
rmpol	429.37		NIST Webbook
rmpol	2520.00		NIST Webbook
rmpol	419.09		NIST Webbook
rmpol	2520.00		NIST Webbook
tb	841.30	K	Joback Method
tc	1121.29	K	Joback Method
tf	577.86	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.79	J/mol×K	841.30	Joback Method
cpg	552.45	J/mol×K	887.97	Joback Method
cpg	564.92	J/mol×K	934.63	Joback Method
cpg	576.29	J/mol×K	981.30	Joback Method
cpg	586.69	J/mol×K	1027.96	Joback Method
cpg	596.25	J/mol×K	1074.63	Joback Method
cpg	605.06	J/mol×K	1121.29	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=C2498660&Units=SI>

Legend

chs:	Standard solid enthalpy of combustion
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
hsub:	Enthalpy of sublimation 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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