5,12-Naphthacenedione

Other names:	5,12-Naphthacenequinone
	Naphthacene-6,11-quinone
	Naphthacenequinone
	5,12-Tetracenequinone
	Naphthacene-5,12-dione
Inchi:	InChI=1S/C18H10O2/c19-17-13-7-3-4-8-14(13)18(20)16-10-12-6-2-1-5-11(12)9-15(16)17
InchiKey:	LZPBKINTWROMEA-UHFFFAOYSA-N
Formula:	C18H10O2
SMILES:	O=C1c2ccccc2C(=O)c2cc3ccccc3cc21
Mol. weight [g/mol]:	258.27
CAS:	1090-13-7

Physical Properties

Property code	Value	Unit	Source
chs	-8368.92	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	109.00	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	2595.00		NIST Webbook
rinpol	428.00		NIST Webbook
rinpol	426.25		NIST Webbook
rinpol	430.57		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	841.30	K	Joback Method
tc	1121.29	K	Joback Method
tf	577.86	K	Joback Method
vc	0.730	m3/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=C1090137&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume