9,10-Phenanthrenedione

Other names:	9,10-Phenanthraquinone
	9,10-Phenanthroquinone
	9,10-phenanthrenequinone
	Phenanthraquinone
	Phenanthroquinone
	phenanthrene, 9,10-dihydro-9,10-dioxo-
	phenanthrenequinone
Inchi:	InChI=1S/C14H8O2/c15-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(13)16/h1-8H
InchiKey:	YYVYAPXYZVYDHN-UHFFFAOYSA-N
Formula:	C14H8O2
SMILES:	O=C1C(=O)c2ccccc2-c2ccccc21
Mol. weight [g/mol]:	208.21
CAS:	84-11-7

Physical Properties

Property code	Value	Unit	Source
chs	-6421.16	kJ/mol	NIST Webbook
chs	-6497.80 ± 1.60	kJ/mol	NIST Webbook
chs	-6460.10	kJ/mol	NIST Webbook
gf	107.94	kJ/mol	Joback Method
hf	-46.60 ± 2.80	kJ/mol	NIST Webbook
hfs	-154.70 ± 2.40	kJ/mol	NIST Webbook
hfus	17.50	kJ/mol	Joback Method
hsub	91.60	kJ/mol	NIST Webbook
hsub	108.10	kJ/mol	NIST Webbook
hsub	108.10 ± 1.50	kJ/mol	NIST Webbook
hvap	61.18	kJ/mol	Joback Method
ie	8.64 ± 0.03	eV	NIST Webbook
log10ws	-4.45		Crippen Method
logp	2.733		Crippen Method
mcvol	152.880	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	362.04		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	360.30		NIST Webbook
rinpol	362.70		NIST Webbook
rinpol	362.70		NIST Webbook

tb	725.82	K	Joback Method
tc	1001.05	K	Joback Method
tf	481.15 ± 4.00	K	NIST Webbook
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.54	J/mol×K	725.82	Joback Method
cpg	415.60	J/mol×K	771.69	Joback Method
cpg	428.41	J/mol×K	817.56	Joback Method
cpg	440.03	J/mol×K	863.44	Joback Method
cpg	450.50	J/mol×K	909.31	Joback Method
cpg	459.88	J/mol×K	955.18	Joback Method
cpg	468.21	J/mol×K	1001.05	Joback Method
hsubt	108.10	kJ/mol	289.00	NIST Webbook
hsubt	132.00	kJ/mol	383.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of Oxygenated Aromatic Solids in Pressurized Hot Water:	https://www.doi.org/10.1021/je800707x
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=C84117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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