

6,13-Pentacenedione

Other names:	6,13-Pentacenequinone
Inchi:	InChI=1S/C22H12O2/c23-21-17-9-13-5-1-2-6-14(13)10-18(17)22(24)20-12-16-8-4-3-7-15
InchiKey:	UFCVADNIXDUEFZ-UHFFFAOYSA-N
Formula:	C22H12O2
SMILES:	O=C1c2cc3ccccc3cc2C(=O)c2cc3ccccc3cc21
Mol. weight [g/mol]:	308.33
CAS:	3029-32-1

Physical Properties

Property code	Value	Unit	Source
chs	-10299.30 ± 6.30	kJ/mol	NIST Webbook
gf	369.34	kJ/mol	Joback Method
hf	135.81	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hsub	116.00	kJ/mol	NIST Webbook
hsub	116.30 ± 5.90	kJ/mol	NIST Webbook
hvap	83.59	kJ/mol	Joback Method
ie	8.07 ± 0.05	eV	NIST Webbook
log10ws	-7.24		Crippen Method
logp	4.768		Crippen Method
mvol	226.680	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
tb	956.78	K	Joback Method
tc	1240.19	K	Joback Method
tf	668.16	K	Joback Method
vc	0.875	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.70	J/mol×K	956.78	Joback Method
cpg	694.22	J/mol×K	1004.01	Joback Method
cpg	706.93	J/mol×K	1051.25	Joback Method
cpg	718.99	J/mol×K	1098.48	Joback Method

cpg	730.61	J/mol×K	1145.72	Joback Method
cpg	741.96	J/mol×K	1192.95	Joback Method
cpg	753.25	J/mol×K	1240.19	Joback Method

Sources

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=C3029321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/25-954-5/6-13-Pentacenedione.pdf>

Generated by Cheméo on 2024-04-23 18:42:43.702360246 +0000 UTC m=+16187012.622937558.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.