1,2-Acenaphthylenedione

Other names:	Acenaphthenedione
	Acenaphthenequinone
	Acenaphthoquinone
	1,2-Acenaphthenedione
	1,2-Acenaphthenequinone
	1,2-Acenaphthalenedione
	Acenaphthylene-1,2-dione
Inchi:	InChI=1S/C12H6O2/c13-11-8-5-1-3-7-4-2-6-9(10(7)8)12(11)14/h1-6H
InchiKey:	AFPRJLBZLPBTPZ-UHFFFAOYSA-N
Formula:	C12H6O2
SMILES:	O=C1C(=O)c2cccc3cccc1c23
Mol. weight [g/mol]:	182.17
CAS:	82-86-0

Physical Properties

Property code	Value	Unit	Source
gf	85.34	kJ/mol	Joback Method
hf	-62.45	kJ/mol	Joback Method
hfus	15.30	kJ/mol	Joback Method
hvap	56.09	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	8.77 ± 0.05	eV	NIST Webbook
log10ws	-3.65		Crippen Method
logp	2.219		Crippen Method
mcvol	129.000	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	314.10		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	313.60		NIST Webbook
tb	672.36	K	Joback Method
tc	940.56	K	Joback Method
tf	525.15 ± 4.00	K	NIST Webbook
tf	533.65 ± 2.00	K	NIST Webbook
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.75	J/mol×K	672.36	Joback Method
cpg	334.08	J/mol×K	717.06	Joback Method
cpg	345.45	J/mol×K	761.76	Joback Method
cpg	355.93	J/mol×K	806.46	Joback Method
cpg	365.59	J/mol×K	851.16	Joback Method
cpg	374.48	J/mol×K	895.86	Joback Method
cpg	382.67	J/mol×K	940.56	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=C82860&Units=SI

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
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