

1,4-Anthracenedione

Other names:	1,4-Anthraquinone 1,4-Anthracenequinone
Inchi:	InChI=1S/C14H8O2/c15-13-5-6-14(16)12-8-10-4-2-1-3-9(10)7-11(12)13/h1-8H
InchiKey:	LSOTZYUVGZKSHR-UHFFFAOYSA-N
Formula:	C14H8O2
SMILES:	O=C1C=CC(=O)c2cc3ccccc3cc21
Mol. weight [g/mol]:	208.21
CAS:	635-12-1

Physical Properties

Property code	Value	Unit	Source
gf	107.94	kJ/mol	Joback Method
hf	-58.27	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	61.18	kJ/mol	Joback Method
ie	8.45 ± 0.02	eV	NIST Webbook
log10ws	-4.34		Crippen Method
logp	2.775		Crippen Method
mvol	152.880	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	328.50		NIST Webbook
rinpol	328.50		NIST Webbook
tb	725.82	K	Joback Method
tc	1001.05	K	Joback Method
tf	487.56	K	Joback Method
vc	0.584	m ³ /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

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=C635121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rropol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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