

9,10-Anthracenedione, 1,5-dichloro-

Other names:	Anthraquinone, 1,5-dichloro- 1,5-Dichloro-9,10-anthraquinone 1,5-Dichloroanthraquinone 1,5-Dichloranthrachinon
Inchi:	InChI=1S/C14H6Cl2O2/c15-9-5-1-3-7-11(9)14(18)8-4-2-6-10(16)12(8)13(7)17/h1-6H
InchiKey:	MQIUMARJCOGCIM-UHFFFAOYSA-N
Formula:	C14H6Cl2O2
SMILES:	O=C1c2cccc(Cl)c2C(=O)c2cccc(Cl)c21
Mol. weight [g/mol]:	277.10
CAS:	82-46-2

Physical Properties

Property code	Value	Unit	Source
gf	64.82	kJ/mol	Joback Method
hf	-112.69	kJ/mol	Joback Method
hfus	25.12	kJ/mol	Joback Method
hvap	71.27	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	3.769		Crippen Method
mcvol	177.360	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	810.64	K	Joback Method
tc	1089.47	K	Joback Method
tf	572.44	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.85	J/molxK	810.64	Joback Method
cpg	451.04	J/molxK	857.11	Joback Method
cpg	461.10	J/molxK	903.58	Joback Method
cpg	470.05	J/molxK	950.06	Joback Method
cpg	477.94	J/molxK	996.53	Joback Method

cpg	484.80	J/mol×K	1043.00	Joback Method
cpg	490.66	J/mol×K	1089.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C82462&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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