1,4-diamino-2,3-dichloro-9,10-antracenedione

Other names: 1,4-diamino-2,3-dichloro-9,10-anthraquinone
1,4-diamino-2,3-dichloroanthraquinone
Inchi: InChI=1S/C14H8Cl2N2O2/c15-9-10(16)12(18)8-7(11(9)17)13(19)5-3-1-2-4-6(5)14(8)20/h
InchiKey: KZYAYVSWIPZDKL-UHFFFAOYSA-N
Formula: C14H8Cl2N2O2
SMILES: Nc1c(Cl)c(Cl)c(N)c2c1C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 307.14

Physical Properties

Property code	Value	Unit	Source
hf	-99.35	kJ/mol	Cheméo Relay (1.0)
hfus	34.74	kJ/mol	Joback Method
ie	8.05	eV	Cheméo Relay (1.0)
log10ws	-5.48		Cheméo Relay (1.0)
logp	2.933		Crippen Method
mcvol	197.320	ml/mol	McGowan Method
tb	696.65	K	Cheméo Relay (1.0)
tf	546.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.09	J/mol×K	965.66	Joback Method
cpg	546.53	J/mol×K	1012.88	Joback Method
cpg	553.75	J/mol×K	1060.10	Joback Method
cpg	559.78	J/mol×K	1107.31	Joback Method
cpg	564.62	J/mol×K	1154.53	Joback Method
cpg	568.29	J/mol×K	1201.75	Joback Method
cpg	570.82	J/mol×K	1248.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Measurement and Correlation of Derivatized Anthraquinone Solubility in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.5b00480
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point