Benzamide, N-(4-chloro-9,10-dihydro-9,10-dioxo-1-anthraceny

Other names: Benzamide, N-(4-chloro-1-anthraquinonyl)-
Anthraquinone, 1-benzamido-4-chloro-
Chlorobenzone
1-Benzamido-4-chloroanthraquinone
1-Benzoylamino-4-chloroanthraquinone
1-Chloro-4-benzamidoanthraquinone
1-Chloro-4-benzoylaminoanthraquinone
1-(Benzoylamino)-2-chloroanthraquinone
1Ba-4-Xa
4-Benzamido-1-chloroanthraquinone
NSC 39954
N-(4-chloro-9,10-dihydro-9,10-dioxo-1-anthryl)benzamide

Inchi: InChI=1S/C21H12ClNO3/c22-15-10-11-16(23-21(26)12-6-2-1-3-7-12)18-17(15)19(24)13-

InchiKey: FNCVZYRPXOZNSM-UHFFFAOYSA-N

Formula: C21H12ClNO3

SMILES: O=C(Nc1ccc(Cl)c2c1C(=O)c1ccccc1C2=O)c1ccccc1

Mol. weight [g/mol]: 361.78

CAS: 81-45-8

Physical Properties

Property code	Value	Unit	Source
gf	208.57	kJ/mol	Joback Method
hf	-64.01	kJ/mol	Joback Method
hfus	39.79	kJ/mol	Joback Method
hvap	97.93	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	4.368		Crippen Method
mcvol	251.540	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
tb	1064.09	K	Joback Method
tc	1343.49	K	Joback Method
tf	750.42	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.03	J/mol×K	1064.09	Joback Method
cpg	761.73	J/mol×K	1110.66	Joback Method
cpg	769.10	J/mol×K	1157.22	Joback Method
cpg	775.26	J/mol×K	1203.79	Joback Method
cpg	780.29	J/mol×K	1250.36	Joback Method
cpg	784.29	J/mol×K	1296.93	Joback Method
cpg	787.35	J/mol×K	1343.49	Joback Method

Sources

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=C81458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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