1-amino-4-(phenylamino)anthraquinone

Other names: 1-Anilino-4-aminoanthraquinone
Inchi: InChI=1S/C20H14N2O2/c21-15-10-11-16(22-12-6-2-1-3-7-12)18-17(15)19(23)13-8-4-5-9
InchiKey: XUDJOVURIXHNRW-UHFFFAOYSA-N
Formula: C20H14N2O2
SMILES: Nc1ccc(Nc2ccccc2)c2c1C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 314.34
CAS: 4395-65-7

Physical Properties

Property code	Value	Unit	Source
gf	407.45	kJ/mol	Joback Method
hf	118.74	kJ/mol	Joback Method
hfus	36.60	kJ/mol	Joback Method
hvap	95.21	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.788		Crippen Method
mcvol	233.620	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
tb	1022.44	K	Joback Method
tc	1304.42	K	Joback Method
tf	742.56	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.40	J/mol×K	1022.44	Joback Method
cpg	742.00	J/mol×K	1069.44	Joback Method
cpg	751.21	J/mol×K	1116.43	Joback Method
cpg	759.13	J/mol×K	1163.43	Joback Method
cpg	765.87	J/mol×K	1210.43	Joback Method
cpg	771.51	J/mol×K	1257.42	Joback Method
cpg	776.17	J/mol×K	1304.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4395657&Units=SI
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

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