Chrysazin, 4-anilino-5-nitro

Other names: 1,8-dihydroxy-4-nitro-5-(phenylamino)anthraquinone
Inchi: InChI=1S/C20H12N2O6/c23-13-8-6-11(21-10-4-2-1-3-5-10)15-17(13)20(26)18-14(24)9-7
InchiKey: DYALWCKAJBVSBZ-UHFFFAOYSA-N
Formula: C20H12N2O6
SMILES: O=C1c2c(O)ccc(Nc3ccccc3)c2C(=O)c2c([N+](=O)[O-])ccc(O)c21
Mol. weight [g/mol]: 376.32
CAS: 20241-76-3

Physical Properties

Property code	Value	Unit	Source
gf	67.31	kJ/mol	Joback Method
hf	-280.43	kJ/mol	Joback Method
hfus	54.33	kJ/mol	Joback Method
hvap	127.19	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.525		Crippen Method
mcvol	252.800	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	1262.99	K	Joback Method
tc	1566.20	K	Joback Method
tf	1026.35	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.44	J/mol×K	1262.99	Joback Method
cpg	891.69	J/mol×K	1313.53	Joback Method
cpg	913.66	J/mol×K	1364.06	Joback Method
cpg	937.69	J/mol×K	1414.60	Joback Method
cpg	964.11	J/mol×K	1465.13	Joback Method
cpg	993.26	J/mol×K	1515.67	Joback Method
cpg	1025.47	J/mol×K	1566.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20241763&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

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