

1-Amino-4-hydroxy-2-phenoxy-9,10-anthraquinone

Other names:

1-Amino-4-hydroxy-2-phenoxyanthraquinone
Anthraquinone, 1-amino-4-hydroxy-2-phenoxy-
Cerven brilantni ostacetova F-LB
Cerven disperzni 60
C.I. Disperse red 60
C.I. Disperse red 71
C.I. Disperse red 83
Disperse polyester pink 2S
Disperse red 60
Dispersol red B 2B
Duranol brilliant red T 2B
Foron brilliant red E 2BL
Hostatherm pink FBL
Latyl cerise N
Miketon polyester red FB
Ostacet brilliant red E-LB
Palanil red bf
Resiren red tb
Resolin red fb
Resolin red fbe
Resorin red fbe
Samaron pink FBL
Serilene brilliant red 2BL
Serilene red 2BL
Sumikaron red E-FBL
Teraprint
Tersetile rubine FL
Transetile Rubine P-FL
1-Amino-4-hydroxy-2-phenoxyanthra-9,10-quinone
1-Amino-4-hydroxy-2-phenoxy-9,10-anthraquinine
1-Amino-4-hydroxy-2-phenoxy-9,10-anthraquinine (Disperse Red 60)

Inchi: InChI=1S/C20H13NO4/c21-18-15(25-11-6-2-1-3-7-11)10-14(22)16-17(18)20(24)13-9-5-4

InchiKey: MHXFEJMQVIWDH-UHFFFAOYSA-N

Formula: C20H13NO4

SMILES: Nc1c(Oc2cccc2)cc(O)c2c1C(=O)c1cccc1C2=O

Mol. weight [g/mol]: 331.33

Physical Properties

Property code	Value	Unit	Source
hf	-265.42	kJ/mol	Cheméo Relay (1.0)
hfus	38.48	kJ/mol	Joback Method
ie	7.53	eV	Cheméo Relay (1.0)
logp	3.542		Crippen Method
mcvol	235.380	ml/mol	McGowan Method
tf	519.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.78	J/mol×K	1075.31	Joback Method
cpg	761.25	J/mol×K	1122.99	Joback Method
cpg	772.00	J/mol×K	1170.68	Joback Method
cpg	782.19	J/mol×K	1218.36	Joback Method
cpg	791.97	J/mol×K	1266.05	Joback Method
cpg	801.47	J/mol×K	1313.73	Joback Method
cpg	810.84	J/mol×K	1361.42	Joback Method
hfust	30.79	kJ/mol	458.20	NIST Webbook
hsubt	152.50	kJ/mol	362.50	NIST Webbook
hsubt	103.80	kJ/mol	413.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C17418585&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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