

1-Amino-2-methyl-4-p-toluidinoanthraquinone

Other names:	1-amino-2-methyl-4-[(4-methylphenyl)amino]anthraquinone 1-Amino-2-methyl-4-[(4-methylphenyl)amino]-9,10-anthraquinone
Inchi:	InChI=1S/C22H18N2O2/c1-12-7-9-14(10-8-12)24-17-11-13(2)20(23)19-18(17)21(25)15-5
InchiKey:	BYGSHXHLDPUXIF-UHFFFAOYSA-N
Formula:	C22H18N2O2
SMILES:	<chem>Cc1ccc(Nc2cc(C)c(N)c3c2C(=O)c2cccc2C3=O)cc1</chem>
Mol. weight [g/mol]:	342.39
CAS:	116-77-8

Physical Properties

Property code	Value	Unit	Source
gf	405.03	kJ/mol	Joback Method
hf	54.52	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	100.99	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	4.405		Crippen Method
mvol	261.800	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
tb	1078.16	K	Joback Method
tc	1353.00	K	Joback Method
tf	790.14	K	Joback Method
vc	0.988	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.98	J/molxK	1078.16	Joback Method
cpg	854.21	J/molxK	1123.97	Joback Method
cpg	862.97	J/molxK	1169.77	Joback Method
cpg	870.33	J/molxK	1215.58	Joback Method
cpg	876.37	J/molxK	1261.38	Joback Method
cpg	881.18	J/molxK	1307.19	Joback Method
cpg	884.81	J/molxK	1353.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116778&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
hsubt:	Enthalpy of sublimation at a given temperature
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

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