

Anthralin

Other names:

9(10H)-Anthracenone, 1,8-dihydroxy-

Anthrone, 1,8-dihydroxy-

1,8-Dihydroxy-9-anthrone

1,8-Dihydroxyanthrone

Anthra-derm

Batridol

Chrysodermol

Cignolin

Cigthranol

Dithranol

Psoriacid-Stift

Batidrol

DrithoCreme

Drithoscalp

Lasan

Psodadrate

Psoriacide

NSC 43970

NSC 629313

1,8-dihydroxyanthracen-9(10H)-one

Inchi:

InChI=1S/C14H10O3/c15-10-5-1-3-8-7-9-4-2-6-11(16)13(9)14(17)12(8)10/h1-6,15-16H,7

InchiKey:

NUZWLKWWNNJHPT-UHFFFAOYSA-N

Formula:

C14H10O3

SMILES:

O=C1c2c(O)cccc2Cc2cccc(O)c21

Mol. weight [g/mol]:

226.23

CAS:

1143-38-0

Physical Properties

Property code	Value	Unit	Source
gf	-78.71	kJ/mol	Joback Method
hf	-275.19	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	82.96	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.233		Crippen Method
mvol	163.050	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method

rmpol	2220.00		NIST Webbook
tb	819.24	K	Joback Method
tc	1094.31	K	Joback Method
tf	642.78	K	Joback Method
vc	0.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.40	J/mol×K	819.24	Joback Method
cpg	478.42	J/mol×K	865.09	Joback Method
cpg	490.26	J/mol×K	910.93	Joback Method
cpg	502.18	J/mol×K	956.78	Joback Method
cpg	514.46	J/mol×K	1002.62	Joback Method
cpg	527.36	J/mol×K	1048.47	Joback Method
cpg	541.15	J/mol×K	1094.31	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=C1143380&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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