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
	1,8-Dihydroxyanthranol
Inchi:	InChI=1S/C14H10O3/c15-10-5-1-3-8-7-9-4-2-6-11(16)13(9)14(17)12(8)10/h1-7,15-17H
InchiKey:	YUTJCNNFTOIOGT-UHFFFAOYSA-N
Formula:	C14H10O3
SMILES:	Oc1cccc2cc3cccc(O)c3c(O)c12
Mol. weight [g/mol]:	226.23
CAS:	480-22-8

Physical Properties

Property code	Value	Unit	Source
gf	-80.78	kJ/mol	Joback Method
hf	-257.02	kJ/mol	Joback Method
hfus	37.05	kJ/mol	Joback Method
hvap	92.02	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.110		Crippen Method

mcvol	163.050	ml/mol	McGowan Method
pc	5836.07	kPa	Joback Method
tb	831.20	K	Joback Method
tc	1104.15	K	Joback Method
tf	687.04	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.68	J/mol×K	831.20	Joback Method
cpg	471.70	J/mol×K	876.69	Joback Method
cpg	483.32	J/mol×K	922.18	Joback Method
cpg	495.94	J/mol×K	967.67	Joback Method
cpg	509.95	J/mol×K	1013.17	Joback Method
cpg	525.78	J/mol×K	1058.66	Joback Method
cpg	543.81	J/mol×K	1104.15	Joback Method
dvisc	0.0000010	Pa×s	687.04	Joback Method
dvisc	0.0000007	Pa×s	711.07	Joback Method
dvisc	0.0000004	Pa×s	735.09	Joback Method
dvisc	0.0000003	Pa×s	759.12	Joback Method
dvisc	0.0000002	Pa×s	783.15	Joback Method
dvisc	0.0000002	Pa×s	807.17	Joback Method
dvisc	0.0000001	Pa×s	831.20	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C480228&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

dvisc:	Dynamic viscosity
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