

9,10-Phenanthrenediol

Inchi:	InChI=1S/C14H10O2/c15-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(13)16/h1-8,15-16H
InchiKey:	ODUSUXJNDWKJKH-UHFFFAOYSA-N
Formula:	C14H10O2
SMILES:	Oc1c(O)c2ccccc2c2ccccc12
Mol. weight [g/mol]:	210.23
CAS:	604-84-2

Physical Properties

Property code	Value	Unit	Source
chs	-6694.80	kJ/mol	NIST Webbook
gf	73.84	kJ/mol	Joback Method
hf	-79.71	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.404		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
tb	750.58	K	Joback Method
tc	1018.90	K	Joback Method
tf	575.32	K	Joback Method
vc	0.487	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.35	J/molxK	750.58	Joback Method
cpg	433.28	J/molxK	795.30	Joback Method
cpg	443.84	J/molxK	840.02	Joback Method
cpg	454.34	J/molxK	884.74	Joback Method
cpg	465.08	J/molxK	929.46	Joback Method
cpg	476.40	J/molxK	974.18	Joback Method
cpg	488.59	J/molxK	1018.90	Joback Method
dvisc	0.0000401	Paxs	575.32	Joback Method

dvisc	0.0000241	Paxs	604.53	Joback Method
dvisc	0.0000152	Paxs	633.74	Joback Method
dvisc	0.0000100	Paxs	662.95	Joback Method
dvisc	0.0000068	Paxs	692.16	Joback Method
dvisc	0.0000048	Paxs	721.37	Joback Method
dvisc	0.0000035	Paxs	750.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C604842&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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

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