

trans-Anthracene-1,2-dihydro-1,2-diol

Inchi:	InChI=1S/C14H12O2/c15-13-6-5-11-7-9-3-1-2-4-10(9)8-12(11)14(13)16/h1-8,13-16H/t13
InchiKey:	UJETWGFPSGKAAS-KBPBESRZSA-N
Formula:	C14H12O2
SMILES:	OC1C=Cc2cc3ccccc3cc2C1O
Mol. weight [g/mol]:	212.24

Physical Properties

Property code	Value	Unit	Source
gf	64.06	kJ/mol	Joback Method
hf	-128.01	kJ/mol	Joback Method
hfus	28.80	kJ/mol	Joback Method
hvap	85.42	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.261		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	2135.00		NIST Webbook
tb	765.20	K	Joback Method
tc	978.77	K	Joback Method
tf	464.28	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.64	J/molxK	765.20	Joback Method
cpg	471.31	J/molxK	800.79	Joback Method
cpg	481.29	J/molxK	836.39	Joback Method
cpg	490.66	J/molxK	871.98	Joback Method
cpg	499.49	J/molxK	907.58	Joback Method
cpg	507.85	J/molxK	943.17	Joback Method
cpg	515.83	J/molxK	978.77	Joback Method
dvisc	0.0012437	Paxs	464.28	Joback Method
dvisc	0.0005307	Paxs	514.43	Joback Method

dvisc	0.0002635	Paxs	564.59	Joback Method
dvisc	0.0001466	Paxs	614.74	Joback Method
dvisc	0.0000892	Paxs	664.89	Joback Method
dvisc	0.0000581	Paxs	715.05	Joback Method
dvisc	0.0000401	Paxs	765.20	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=R109747&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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