trans-Anthracene, 1,2,3,4-tetrahydro-1,2-diol

Inchi: InChI=1S/C14H14O2/c15-13-6-5-11-7-9-3-1-2-4-10(9)8-12(11)14(13)16/h1-4,7-8,13-16H
InchiKey: OCFQOCVMVLZKPR-KBPBESRZSA-N
Formula: C14H14O2
SMILES: OC1CCc2cc3ccccc3cc2C1O
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
gf	34.10	kJ/mol	Joback Method
hf	-185.79	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	85.13	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.180		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	2095.00		NIST Webbook
tb	766.04	K	Joback Method
tc	978.17	K	Joback Method
tf	463.52	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.66	J/mol×K	766.04	Joback Method
cpg	498.25	J/mol×K	801.40	Joback Method
cpg	509.10	J/mol×K	836.75	Joback Method
cpg	519.29	J/mol×K	872.11	Joback Method
cpg	528.89	J/mol×K	907.46	Joback Method
cpg	537.96	J/mol×K	942.82	Joback Method
cpg	546.59	J/mol×K	978.17	Joback Method
dvisc	0.0012923	Pa×s	463.52	Joback Method
dvisc	0.0005368	Pa×s	513.94	Joback Method

dvisc	0.0002609	Pa×s	564.36	Joback Method
dvisc	0.0001427	Pa×s	614.78	Joback Method
dvisc	0.0000855	Pa×s	665.20	Joback Method
dvisc	0.0000551	Pa×s	715.62	Joback Method
dvisc	0.0000376	Pa×s	766.04	Joback Method

Sources

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=R109698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/47-483-4/trans-Anthracene-1-2-3-4-tetrahydro-1-2-diol.pdf
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