

Anthracene transannular peroxide

Inchi:	InChI=1S/C14H10O2/c1-2-6-10-9(5-1)13-11-7-3-4-8-12(11)14(10)16-15-13/h1-8,13-14H
InchiKey:	SRWMCQYMZIZLAY-UHFFFAOYSA-N
Formula:	C14H10O2
SMILES:	c1ccc2c(c1)C1OOC2c2ccccc21
Mol. weight [g/mol]:	210.23
CAS:	220-42-8

Physical Properties

Property code	Value	Unit	Source
chs	-7020.80	kJ/mol	NIST Webbook
gf	246.02	kJ/mol	Joback Method
hf	11.75	kJ/mol	Joback Method
hfs	82.40	kJ/mol	NIST Webbook
hfus	35.75	kJ/mol	Joback Method
hvap	61.14	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.141		Crippen Method
mcvol	150.620	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	641.88	K	Joback Method
tc	895.06	K	Joback Method
tf	421.48	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.48	J/molxK	641.88	Joback Method
cpg	412.96	J/molxK	684.08	Joback Method
cpg	426.17	J/molxK	726.27	Joback Method
cpg	438.29	J/molxK	768.47	Joback Method
cpg	449.51	J/molxK	810.66	Joback Method
cpg	459.99	J/molxK	852.86	Joback Method
cpg	469.93	J/molxK	895.06	Joback Method

dvisc	0.0029382	Paxs	421.48	Joback Method
dvisc	0.0026272	Paxs	458.21	Joback Method
dvisc	0.0023884	Paxs	494.95	Joback Method
dvisc	0.0022001	Paxs	531.68	Joback Method
dvisc	0.0020483	Paxs	568.41	Joback Method
dvisc	0.0019235	Paxs	605.15	Joback Method
dvisc	0.0018194	Paxs	641.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C220428&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

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
hfs:	Solid phase 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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