9,10-Dihyro-9,10,11-trimethyl-9,10-methanoanthra

Inchi: InChI=1S/C18H18O/c1-17-12-7-3-5-9-14(12)18(2,16(17)11-19)15-10-6-4-8-13(15)17/h3-
InchiKey: JJHQPXQWPGFQHQ-AYHJJNSGSA-N
Formula: C18H18O
SMILES: CC12c3ccccc3C(C)(c3ccccc31)C2CO
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	308.53	kJ/mol	Joback Method
hf	57.26	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	74.92	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.234		Crippen Method
mcvol	201.110	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	3036.00		NIST Webbook
tb	763.22	K	Joback Method
tc	992.06	K	Joback Method
tf	521.32	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.26	J/mol×K	763.22	Joback Method
cpg	606.79	J/mol×K	801.36	Joback Method
cpg	622.51	J/mol×K	839.50	Joback Method
cpg	638.79	J/mol×K	877.64	Joback Method
cpg	655.99	J/mol×K	915.78	Joback Method
cpg	674.45	J/mol×K	953.92	Joback Method
cpg	694.54	J/mol×K	992.06	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419262&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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