9,10-Dihydro-9,10-ethanoanthracene-11,11,12,12-t

Inchi: InChI=1S/C20H10N4/c21-9-19(10-22)17-13-5-1-2-6-14(13)18(20(19,11-23)12-24)16-8-4-
InchiKey: BZIGFCWZJSWLLX-UHFFFAOYSA-N
Formula: C20H10N4
SMILES: N#CC1(C#N)C2c3ccccc3C(c3ccccc32)C1(C#N)C#N
Mol. weight [g/mol]: 306.32
CAS: 1625-84-9

Physical Properties

Property code	Value	Unit	Source
gf	975.10	kJ/mol	Joback Method
hf	801.23	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	104.46	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.345		Crippen Method
mcvol	228.940	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
tb	1124.72	K	Joback Method
tc	1405.38	K	Joback Method
tf	735.24	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.20	J/mol×K	1124.72	Joback Method
cpg	809.03	J/mol×K	1171.50	Joback Method
cpg	849.95	J/mol×K	1218.27	Joback Method
cpg	896.56	J/mol×K	1265.05	Joback Method
cpg	949.48	J/mol×K	1311.83	Joback Method
cpg	1009.32	J/mol×K	1358.61	Joback Method
cpg	1076.71	J/mol×K	1405.38	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=C1625849&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
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