4a,8a-Ethenonaphthalene, 1,2,3,4,5,8-hexahydro-

Inchi: InChI=1S/C12H16/c1-2-6-12-8-4-3-7-11(12,5-1)9-10-12/h1-2,9-10H,3-8H2
InchiKey: CZKPIMSROUSLTQ-UHFFFAOYSA-N
Formula: C12H16
SMILES: C1=CCC23C=CC2(C1)CCCC3
Mol. weight [g/mol]: 160.26
CAS: 24139-32-0

Physical Properties

Property code	Value	Unit	Source
gf	252.76	kJ/mol	Joback Method
hf	75.29	kJ/mol	Joback Method
hfus	3.72	kJ/mol	Joback Method
hvap	41.15	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-3.75		Crippen Method
logp	3.453		Crippen Method
mcvol	138.760	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	510.46	K	Joback Method
tc	760.27	K	Joback Method
tf	321.82	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.36	J/mol×K	510.46	Joback Method
cpg	355.33	J/mol×K	552.10	Joback Method
cpg	374.10	J/mol×K	593.73	Joback Method
cpg	391.10	J/mol×K	635.37	Joback Method
cpg	406.73	J/mol×K	677.00	Joback Method
cpg	421.43	J/mol×K	718.64	Joback Method
cpg	435.61	J/mol×K	760.27	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=C24139320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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