

4a,8a-Ethenonaphthalene, 1,2,3,4-tetrahydro-

Inchi:	InChI=1S/C12H14/c1-2-6-12-8-4-3-7-11(12,5-1)9-10-12/h1-2,5-6,9-10H,3-4,7-8H2
InchiKey:	PATIUEOBXCLCSQ-UHFFFAOYSA-N
Formula:	C12H14
SMILES:	C1=CC23C=CC2(C=C1)CCCC3
Mol. weight [g/mol]:	158.24
CAS:	24139-33-1

Physical Properties

Property code	Value	Unit	Source
gf	282.72	kJ/mol	Joback Method
hf	133.07	kJ/mol	Joback Method
hfus	4.94	kJ/mol	Joback Method
hvap	41.44	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	3.229		Crippen Method
mcvol	134.460	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	509.62	K	Joback Method
tc	762.15	K	Joback Method
tf	322.58	K	Joback Method
vc	0.509	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.01	J/molxK	509.62	Joback Method
cpg	336.61	J/molxK	551.71	Joback Method
cpg	354.02	J/molxK	593.80	Joback Method
cpg	369.69	J/molxK	635.89	Joback Method
cpg	384.05	J/molxK	677.98	Joback Method
cpg	397.54	J/molxK	720.06	Joback Method
cpg	410.59	J/molxK	762.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24139331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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