1,4-Ethenoanthracene, 1,4-dihydro-

Other names: 2,3-Naphthobarrelene
1,4-Dihydro-1,4-ethenoanthracene
Inchi: InChI=1S/C16H12/c1-2-4-14-10-16-12-7-5-11(6-8-12)15(16)9-13(14)3-1/h1-12H
InchiKey: FSVHOWXJQOZKEV-UHFFFAOYSA-N
Formula: C16H12
SMILES: C1=CC2C=CC1c1cc3ccccc3cc12
Mol. weight [g/mol]: 204.27
CAS: 27765-96-4

Physical Properties

Property code	Value	Unit	Source
gf	465.06	kJ/mol	Joback Method
hf	292.25	kJ/mol	Joback Method
hfus	26.19	kJ/mol	Joback Method
hvap	56.86	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.147		Crippen Method
mcvol	162.760	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	342.20		NIST Webbook
rinpol	342.20		NIST Webbook
rinpol	335.80		NIST Webbook
rinpol	336.60		NIST Webbook
tb	632.90	K	Joback Method
tc	885.04	K	Joback Method
tf	391.64	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.03	J/mol×K	632.90	Joback Method
cpg	433.27	J/mol×K	674.92	Joback Method
cpg	448.10	J/mol×K	716.95	Joback Method

cpg	461.71	J/mol×K	758.97	Joback Method
cpg	474.32	J/mol×K	800.99	Joback Method
cpg	486.11	J/mol×K	843.02	Joback Method
cpg	497.28	J/mol×K	885.04	Joback Method
dvisc	0.0020859	Pa×s	391.64	Joback Method
dvisc	0.0019762	Pa×s	431.85	Joback Method
dvisc	0.0018896	Pa×s	472.06	Joback Method
dvisc	0.0018196	Pa×s	512.27	Joback Method
dvisc	0.0017618	Pa×s	552.48	Joback Method
dvisc	0.0017133	Pa×s	592.69	Joback Method
dvisc	0.0016721	Pa×s	632.90	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=C27765964&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
dvisc:	Dynamic viscosity
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