

Anthracene, 9-ethenyl-

Other names:	9-Vinylanthracene 9-Ethenyl anthracene
Inchi:	InChI=1S/C16H12/c1-2-14-15-9-5-3-7-12(15)11-13-8-4-6-10-16(13)14/h2-11H,1H2
InchiKey:	OGOYZCQQFAGRI-UHFFFAOYSA-N
Formula:	C16H12
SMILES:	<chem>C=Cc1c2ccccc2cc2ccccc12</chem>
Mol. weight [g/mol]:	204.27
CAS:	2444-68-0

Physical Properties

Property code	Value	Unit	Source
gf	478.13	kJ/mol	Joback Method
hf	347.59	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	57.42	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.636		Crippen Method
mvol	169.320	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	311.70		NIST Webbook
rinpol	334.13		NIST Webbook
rinpol	334.63		NIST Webbook
rinpol	336.76		NIST Webbook
rinpol	311.60		NIST Webbook
rinpol	311.60		NIST Webbook
tb	636.76	K	Joback Method
tc	885.82	K	Joback Method
tf	385.18	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.65	J/molxK	636.76	Joback Method

cpg	423.79	J/molxK	678.27	Joback Method
cpg	437.69	J/molxK	719.78	Joback Method
cpg	450.50	J/molxK	761.29	Joback Method
cpg	462.36	J/molxK	802.80	Joback Method
cpg	473.41	J/molxK	844.31	Joback Method
cpg	483.79	J/molxK	885.82	Joback Method
dvisc	0.0013633	Paxs	385.18	Joback Method
dvisc	0.0010332	Paxs	427.11	Joback Method
dvisc	0.0008229	Paxs	469.04	Joback Method
dvisc	0.0006803	Paxs	510.97	Joback Method
dvisc	0.0005789	Paxs	552.90	Joback Method
dvisc	0.0005039	Paxs	594.83	Joback Method
dvisc	0.0004468	Paxs	636.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.70	K	1.30	NIST Webbook

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=C2444680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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