

Anthracene, 9-propyl-

Inchi:	InChI=1S/C17H16/c1-2-7-17-15-10-5-3-8-13(15)12-14-9-4-6-11-16(14)17/h3-6,8-12H,2,7
InchiKey:	DYERJGPIBJPPKA-UHFFFAOYSA-N
Formula:	C17H16
SMILES:	CCc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	220.31
CAS:	1498-77-7

Physical Properties

Property code	Value	Unit	Source
gf	398.71	kJ/mol	Joback Method
hf	201.52	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.946		Crippen Method
mvol	187.710	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	662.96	K	Joback Method
tc	901.48	K	Joback Method
tf	398.21	K	Joback Method
vc	0.724	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.25	J/molxK	662.96	Joback Method
cpg	497.56	J/molxK	702.71	Joback Method
cpg	512.69	J/molxK	742.47	Joback Method
cpg	526.74	J/molxK	782.22	Joback Method
cpg	539.84	J/molxK	821.98	Joback Method
cpg	552.12	J/molxK	861.73	Joback Method
cpg	563.71	J/molxK	901.48	Joback Method
dvisc	0.0014293	Paxs	398.21	Joback Method
dvisc	0.0010458	Paxs	442.34	Joback Method

dvisc	0.0008099	Paxs	486.46	Joback Method
dvisc	0.0006544	Paxs	530.59	Joback Method
dvisc	0.0005463	Paxs	574.71	Joback Method
dvisc	0.0004680	Paxs	618.84	Joback Method
dvisc	0.0004093	Paxs	662.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1498777&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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