

1,4:5,8:9,10-Trimethanoanthracene, 1,2,3,4,4a,5,8,8a,9,9a,10,10a-dodecahydro-(1 «alph

Inchi:	InChI=1S/C17H22/c1-2-9-5-8(1)14-12-7-13(15(9)14)17-11-4-3-10(6-11)16(12)17/h1-2,8-
InchiKey:	FUCGLOJSPSEIKX-JDEKWYGUSA-N
Formula:	C17H22
SMILES:	C1=CC2CC1C1C3CC(C21)C1C2CCC(C2)C31
Mol. weight [g/mol]:	226.36
CAS:	87424-91-7

Physical Properties

Property code	Value	Unit	Source
gf	467.98	kJ/mol	Joback Method
hf	25.17	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Joback Method
ie	8.68	eV	NIST Webbook
log10ws	-3.74		Crippen Method
logp	3.737		Crippen Method
mcvol	180.930	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
tb	605.01	K	Joback Method
tc	828.43	K	Joback Method
tf	376.31	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.82	J/molxK	605.01	Joback Method
cpg	676.51	J/molxK	791.19	Joback Method
cpg	658.01	J/molxK	753.95	Joback Method
cpg	638.31	J/molxK	716.72	Joback Method
cpg	617.19	J/molxK	679.48	Joback Method
cpg	594.43	J/molxK	642.25	Joback Method
cpg	694.04	J/molxK	828.43	Joback Method
dvisc	0.0627123	Paxs	605.01	Joback Method

dvisc	0.0475853	Paxs	566.89	Joback Method
dvisc	0.0346984	Paxs	528.78	Joback Method
dvisc	0.0240900	Paxs	490.66	Joback Method
dvisc	0.0157277	Paxs	452.54	Joback Method
dvisc	0.0094937	Paxs	414.43	Joback Method
dvisc	0.0051736	Paxs	376.31	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=C87424917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	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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