

1,4:5,8:9,10-Trimethanoanthracene, 1,4,4a,5,8,8a,9,9a,10,10a-decahydro-(1 «alpha»,4 «a

Inchi:	InChI=1S/C17H20/c1-2-9-5-8(1)14-12-7-13(15(9)14)17-11-4-3-10(6-11)16(12)17/h1-4,8-
InchiKey:	KVHGVQIXSZOTQM-SKDQRCGVSA-N
Formula:	C17H20
SMILES:	C1=CC2CC1C1C3CC(C21)C1C2C=CC(C2)C31
Mol. weight [g/mol]:	224.34
CAS:	50415-43-5

Physical Properties

Property code	Value	Unit	Source
gf	497.94	kJ/mol	Joback Method
hf	82.95	kJ/mol	Joback Method
hfus	37.42	kJ/mol	Joback Method
hvap	52.09	kJ/mol	Joback Method
ie	8.24	eV	NIST Webbook
log10ws	-3.60		Crippen Method
logp	3.513		Crippen Method
mcvol	176.630	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
tb	604.17	K	Joback Method
tc	829.70	K	Joback Method
tf	377.07	K	Joback Method
vc	0.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.75	J/molxK	604.17	Joback Method
cpg	572.31	J/molxK	641.76	Joback Method
cpg	594.03	J/molxK	679.35	Joback Method
cpg	614.14	J/molxK	716.93	Joback Method
cpg	632.87	J/molxK	754.52	Joback Method
cpg	650.45	J/molxK	792.11	Joback Method
cpg	667.09	J/molxK	829.70	Joback Method
dvisc	0.0048840	Paxs	377.07	Joback Method

dvisc	0.0091159	Paxs	414.92	Joback Method
dvisc	0.0153287	Paxs	452.77	Joback Method
dvisc	0.0237898	Paxs	490.62	Joback Method
dvisc	0.0346681	Paxs	528.47	Joback Method
dvisc	0.0480408	Paxs	566.32	Joback Method
dvisc	0.0639055	Paxs	604.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50415435&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

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
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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