

Benz(a)anthracene, 7,8-dimethyl-

Other names:	5,10-Dimethyl-1,2-benzanthracene 7,8-Dimethylbenz(a)anthracene
Inchi:	InChI=1S/C20H16/c1-13-6-5-8-16-12-19-17(14(2)20(13)16)11-10-15-7-3-4-9-18(15)19/h
InchiKey:	VKXBZRGZQZQJJW-UHFFFAOYSA-N
Formula:	C20H16
SMILES:	Cc1cccc2cc3c(ccc4cccc43)c(C)c12
Mol. weight [g/mol]:	256.34
CAS:	604-81-9

Physical Properties

Property code	Value	Unit	Source
gf	511.36	kJ/mol	Joback Method
hf	307.73	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	69.96	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	5.763		Crippen Method
mvol	210.520	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
tb	760.54	K	Joback Method
tc	1013.66	K	Joback Method
tf	489.76	K	Joback Method
vc	0.814	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.63	J/molxK	760.54	Joback Method
cpg	586.13	J/molxK	802.73	Joback Method
cpg	600.62	J/molxK	844.91	Joback Method
cpg	614.28	J/molxK	887.10	Joback Method
cpg	627.28	J/molxK	929.28	Joback Method
cpg	639.81	J/molxK	971.47	Joback Method
cpg	652.05	J/molxK	1013.66	Joback Method

dvisc	0.0014862	Paxs	489.76	Joback Method
dvisc	0.0012234	Paxs	534.89	Joback Method
dvisc	0.0010381	Paxs	580.02	Joback Method
dvisc	0.0009019	Paxs	625.15	Joback Method
dvisc	0.0007987	Paxs	670.28	Joback Method
dvisc	0.0007181	Paxs	715.41	Joback Method
dvisc	0.0006539	Paxs	760.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C604819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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