

Benz(a)anthracene, 12-ethyl-

Other names:	12-Ethylbenz(a)anthracene
Inchi:	InChI=1S/C20H16/c1-2-17-18-9-5-4-8-15(18)13-16-12-11-14-7-3-6-10-19(14)20(16)17/h3
InchiKey:	ZZIFQBYIKWXEHJ-UHFFFAOYSA-N
Formula:	C20H16
SMILES:	CCc1c2ccccc2cc2ccc3ccccc3c12
Mol. weight [g/mol]:	256.34
CAS:	18868-66-1

Physical Properties

Property code	Value	Unit	Source
gf	520.99	kJ/mol	Joback Method
hf	319.20	kJ/mol	Joback Method
hfus	31.49	kJ/mol	Joback Method
hvap	69.30	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	5.709		Crippen Method
mcvol	210.520	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
tb	755.56	K	Joback Method
tc	1007.92	K	Joback Method
tf	477.24	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.83	J/mol×K	755.56	Joback Method
cpg	587.44	J/mol×K	797.62	Joback Method
cpg	601.99	J/mol×K	839.68	Joback Method
cpg	615.68	J/mol×K	881.74	Joback Method
cpg	628.69	J/mol×K	923.80	Joback Method
cpg	641.21	J/mol×K	965.86	Joback Method
cpg	653.44	J/mol×K	1007.92	Joback Method
dvisc	0.0016002	Pa×s	477.24	Joback Method

dvisc	0.0012852	Pa×s	523.63	Joback Method
dvisc	0.0010698	Pa×s	570.01	Joback Method
dvisc	0.0009154	Pa×s	616.40	Joback Method
dvisc	0.0008006	Pa×s	662.79	Joback Method
dvisc	0.0007125	Pa×s	709.17	Joback Method
dvisc	0.0006433	Pa×s	755.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18868661&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

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
mccvol:	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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