

Benz[a]anthracene, 7-ethyl-

Other names:	10-Ethyl-1,2-benzanthracene 7-Ethylbenz[a]anthracene
Inchi:	InChI=1S/C20H16/c1-2-16-18-10-6-4-8-15(18)13-20-17-9-5-3-7-14(17)11-12-19(16)20/h
InchiKey:	HBFJJKFTOQAJHO-UHFFFAOYSA-N
Formula:	C20H16
SMILES:	CCc1c2ccccc2cc2c1ccc1ccccc12
Mol. weight [g/mol]:	256.34
CAS:	3697-30-1

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.83	J/molxK	755.56	Joback Method
cpg	641.21	J/molxK	965.86	Joback Method
cpg	628.69	J/molxK	923.80	Joback Method
cpg	615.68	J/molxK	881.74	Joback Method
cpg	601.99	J/molxK	839.68	Joback Method
cpg	587.44	J/molxK	797.62	Joback Method
cpg	653.44	J/molxK	1007.92	Joback Method

dvisc	0.0006433	Paxs	755.56	Joback Method
dvisc	0.0007125	Paxs	709.17	Joback Method
dvisc	0.0008006	Paxs	662.79	Joback Method
dvisc	0.0009154	Paxs	616.40	Joback Method
dvisc	0.0010698	Paxs	570.01	Joback Method
dvisc	0.0012852	Paxs	523.63	Joback Method
dvisc	0.0016002	Paxs	477.24	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=C3697301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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