12-Ethylbenz[a]anthracene

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]: 256.35

Physical Properties

Property code	Value	Unit	Source
af	0.5792		Cheméo Relay (1.0)
hf	245.34	kJ/mol	Cheméo Relay (1.0)
hfus	31.49	kJ/mol	Joback Method
hvap	111.06	kJ/mol	Cheméo Relay (1.0)
ie	7.27	eV	Cheméo Relay (1.0)
log10ws	-7.42		Cheméo Relay (1.0)
logp	5.709		Crippen Method
mcvol	210.520	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
tb	721.17	K	Cheméo Relay (1.0)
tc	999.19	K	Cheméo Relay (1.0)
tf	384.89	K	Cheméo Relay (1.0)
vc	0.790	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18868661&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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