7-Ethyl-12-methylbenz[a]anthracene

Other names: 7-Ethyl-12-methylbenz(a)anthracene
Inchi: InChI=1S/C21H18/c1-3-16-19-11-7-6-9-17(19)14(2)21-18-10-5-4-8-15(18)12-13-20(16)21
InchiKey: KGHAOMPXHGIHAL-UHFFFAOYSA-N
Formula: C21H18
SMILES: CCc1c2ccccc2c(C)c2c1ccc1ccccc12
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
af	0.6091		Cheméo Relay (1.0)
hf	208.33	kJ/mol	Cheméo Relay (1.0)
hfus	33.69	kJ/mol	Joback Method
hvap	116.64	kJ/mol	Cheméo Relay (1.0)
ie	7.31	eV	Cheméo Relay (1.0)
log10ws	-7.53		Cheméo Relay (1.0)
logp	6.017		Crippen Method
mcvol	224.610	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
tb	727.83	K	Cheméo Relay (1.0)
tc	1005.51	K	Cheméo Relay (1.0)
tf	387.04	K	Cheméo Relay (1.0)
vc	0.845	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.02	J/mol×K	783.42	Joback Method
cpg	640.91	J/mol×K	824.72	Joback Method
cpg	655.84	J/mol×K	866.03	Joback Method
cpg	669.98	J/mol×K	907.33	Joback Method
cpg	683.49	J/mol×K	948.64	Joback Method
cpg	696.57	J/mol×K	989.94	Joback Method
cpg	709.36	J/mol×K	1031.24	Joback Method
dvisc	0.0014719	Pa×s	501.03	Joback Method

dvisc	0.0011934	Pa×s	548.10	Joback Method
dvisc	0.0010003	Pa×s	595.16	Joback Method
dvisc	0.0008604	Pa×s	642.23	Joback Method
dvisc	0.0007555	Pa×s	689.29	Joback Method
dvisc	0.0006744	Pa×s	736.36	Joback Method
dvisc	0.0006104	Pa×s	783.42	Joback Method

Sources

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
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=C16354500&Units=SI

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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