Benz(a)anthracene, 12-ethyl-7-methyl-

Other names: 12-Ethyl-7-methylbenz(a)anthracene
Inchi: InChI=1S/C21H18/c1-3-16-20-11-7-6-9-17(20)14(2)18-13-12-15-8-4-5-10-19(15)21(16)18
InchiKey: FTMBVQWARWOALX-UHFFFAOYSA-N
Formula: C21H18
SMILES: CCc1c2ccccc2c(C)c2ccc3ccccc3c12
Mol. weight [g/mol]: 270.37
CAS: 16354-55-5

Physical Properties

Property code	Value	Unit	Source
gf	519.78	kJ/mol	Joback Method
hf	287.09	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	72.18	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	6.017		Crippen Method
mcvol	224.610	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
tb	783.42	K	Joback Method
tc	1031.24	K	Joback Method
tf	501.03	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.02	J/mol×K	783.42	Joback Method
cpg	696.57	J/mol×K	989.94	Joback Method
cpg	683.49	J/mol×K	948.64	Joback Method
cpg	669.98	J/mol×K	907.33	Joback Method
cpg	655.84	J/mol×K	866.03	Joback Method
cpg	640.91	J/mol×K	824.72	Joback Method
cpg	709.36	J/mol×K	1031.24	Joback Method
dvisc	0.0006104	Pa×s	783.42	Joback Method

dvisc	0.0006744	Pa×s	736.36	Joback Method
dvisc	0.0007555	Pa×s	689.29	Joback Method
dvisc	0.0008604	Pa×s	642.23	Joback Method
dvisc	0.0010003	Pa×s	595.16	Joback Method
dvisc	0.0011934	Pa×s	548.10	Joback Method
dvisc	0.0014719	Pa×s	501.03	Joback Method

Sources

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=C16354555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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