4,7,12-Trimethylbenz[a]anthracene

Other names: Benz(a)anthracene, 4,7,12-trimethyl-
Inchi: InChI=1S/C21H18/c1-13-7-6-10-20-16(13)11-12-19-14(2)17-8-4-5-9-18(17)15(3)21(19)2
InchiKey: PYUNTMRZRNSDKA-UHFFFAOYSA-N
Formula: C21H18
SMILES: Cc1cccc2c1ccc1c(C)c3ccccc3c(C)c12
Mol. weight [g/mol]: 270.37
CAS: 35187-24-7

Physical Properties

Property code	Value	Unit	Source
gf	510.15	kJ/mol	Joback Method
hf	275.62	kJ/mol	Joback Method
hfus	33.30	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
ie	7.06 ± 0.03	eV	NIST Webbook
log10ws	-8.31		Crippen Method
logp	6.071		Crippen Method
mcvol	224.610	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
tb	788.40	K	Joback Method
tc	1036.95	K	Joback Method
tf	513.55	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.87	J/mol×K	788.40	Joback Method
cpg	639.68	J/mol×K	829.83	Joback Method
cpg	654.57	J/mol×K	871.25	Joback Method
cpg	668.68	J/mol×K	912.68	Joback Method
cpg	682.20	J/mol×K	954.10	Joback Method
cpg	695.27	J/mol×K	995.53	Joback Method
cpg	708.06	J/mol×K	1036.95	Joback Method

dvisc	0.0013788	Pa×s	513.55	Joback Method
dvisc	0.0011437	Pa×s	559.36	Joback Method
dvisc	0.0009759	Pa×s	605.17	Joback Method
dvisc	0.0008516	Pa×s	650.98	Joback Method
dvisc	0.0007565	Pa×s	696.78	Joback Method
dvisc	0.0006819	Pa×s	742.59	Joback Method
dvisc	0.0006221	Pa×s	788.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35187247&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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