

Benz(a)anthracene, 2,7,12-trimethyl-

Other names:	2,7,12-Trimethylbenz(a)anthracene
Inchi:	InChI=1S/C21H18/c1-13-8-9-16-10-11-19-14(2)17-6-4-5-7-18(17)15(3)21(19)20(16)12-1
InchiKey:	ZMRPKSZAJUNIAT-UHFFFAOYSA-N
Formula:	C21H18
SMILES:	<chem>Cc1ccc2ccc3c(C)c4ccccc4c(C)c3c2c1</chem>
Mol. weight [g/mol]:	270.37
CAS:	35215-31-7

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
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.87	J/molxK	788.40	Joback Method
cpg	639.68	J/molxK	829.83	Joback Method
cpg	654.57	J/molxK	871.25	Joback Method
cpg	668.68	J/molxK	912.68	Joback Method
cpg	682.20	J/molxK	954.10	Joback Method
cpg	695.27	J/molxK	995.53	Joback Method
cpg	708.06	J/molxK	1036.95	Joback Method
dvisc	0.0013788	Paxs	513.55	Joback Method

dvisc	0.0011437	Paxs	559.36	Joback Method
dvisc	0.0009759	Paxs	605.17	Joback Method
dvisc	0.0008516	Paxs	650.98	Joback Method
dvisc	0.0007565	Paxs	696.78	Joback Method
dvisc	0.0006819	Paxs	742.59	Joback Method
dvisc	0.0006221	Paxs	788.40	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=C35215317&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

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