

7-Butyl-12-methylbenz[a]anthracene

Inchi:	InChI=1S/C23H22/c1-3-4-10-21-20-13-8-7-11-18(20)16(2)23-19-12-6-5-9-17(19)14-15-2
InchiKey:	PBRXQWATBIWV-FV-UHFFFAOYSA-N
Formula:	C23H22
SMILES:	CCCCc1c2ccccc2c(C)c2c1ccc1ccccc12
Mol. weight [g/mol]:	298.42
CAS:	16354-51-1

Physical Properties

Property code	Value	Unit	Source
gf	536.62	kJ/mol	Joback Method
hf	245.81	kJ/mol	Joback Method
hfus	38.87	kJ/mol	Joback Method
hvap	76.64	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	6.797		Crippen Method
mvol	252.790	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	829.18	K	Joback Method
tc	1068.08	K	Joback Method
tf	523.57	K	Joback Method
vc	0.982	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.06	J/molxK	829.18	Joback Method
cpg	812.84	J/molxK	1028.27	Joback Method
cpg	798.77	J/molxK	988.45	Joback Method
cpg	784.32	J/molxK	948.63	Joback Method
cpg	769.33	J/molxK	908.81	Joback Method
cpg	753.63	J/molxK	869.00	Joback Method
cpg	826.68	J/molxK	1068.08	Joback Method
dvisc	0.0005210	Paxs	829.18	Joback Method
dvisc	0.0005824	Paxs	778.25	Joback Method

dvisc	0.0006613	Paxs	727.31	Joback Method
dvisc	0.0007654	Paxs	676.38	Joback Method
dvisc	0.0009072	Paxs	625.44	Joback Method
dvisc	0.0011082	Paxs	574.51	Joback Method
dvisc	0.0014075	Paxs	523.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16354511&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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