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)14-15-22
InchiKey: PBRXQWATBIWVFV-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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0006613	Pa×s	727.31	Joback Method
dvisc	0.0007654	Pa×s	676.38	Joback Method
dvisc	0.0009072	Pa×s	625.44	Joback Method
dvisc	0.0011082	Pa×s	574.51	Joback Method
dvisc	0.0014075	Pa×s	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/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
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