

Benzo[tuv]naphtho[2,1-b]picene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C32H18/c1-3-7-23-19(5-1)9-13-25-27-15-12-22-18-30-24-8-4-2-6-20(24)10-14

BTQFMWRJXYLATA-UHFFFAOYSA-N

C32H18

c1ccc2c(c1)ccc1c2cc2ccc3c4ccc5ccccc5c4cc4ccc1c2c43

402.49

119123-35-2

Physical Properties

Property code	Value	Unit	Source
gf	1013.98	kJ/mol	Joback Method
hf	755.93	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	103.92	kJ/mol	Joback Method
log10ws	-13.52		Crippen Method
logp	9.197		Crippen Method
mcvol	306.060	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	1113.28	K	Joback Method
tc	1393.93	K	Joback Method
tf	787.12	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.19	J/mol×K	1113.28	Joback Method
cpg	1141.24	J/mol×K	1347.16	Joback Method
cpg	1101.51	J/mol×K	1300.38	Joback Method
cpg	1066.07	J/mol×K	1253.61	Joback Method
cpg	1034.40	J/mol×K	1206.83	Joback Method
cpg	1005.95	J/mol×K	1160.06	Joback Method
cpg	1185.80	J/mol×K	1393.93	Joback Method
dvisc	0.0110928	Pa×s	1113.28	Joback Method
dvisc	0.0114227	Pa×s	1058.92	Joback Method

dvisc	0.0117997	Pa×s	1004.56	Joback Method
dvisc	0.0122346	Pa×s	950.20	Joback Method
dvisc	0.0127414	Pa×s	895.84	Joback Method
dvisc	0.0133389	Pa×s	841.48	Joback Method
dvisc	0.0140531	Pa×s	787.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119123352&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

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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