Tetranaphtho[3,2,1-de:1',2',3'-jk:3",2",

Other names: Tetranaphtho[3,2,1-de:1',2',3'-jk:3",2",1"-op:1"',2"',3"'-uv)pentacene
Inchi: InChI=1S/C50H26/c1-5-13-35-27(9-1)21-31-17-18-32-22-28-10-2-6-14-36(28)48-40-26-4
InchiKey: MRRUILGWVZWLSV-UHFFFAOYSA-N
Formula: C50H26
SMILES: c1ccc2c(c1)cc1ccc3cc4ccccc4c4c5cc6c(cc5c2c1c34)c1c2ccccc2cc2ccc3cc4ccccc4c6c3
Mol. weight [g/mol]: 626.74
CAS: 72382-92-4

Physical Properties

Property code	Value	Unit	Source
gf	1644.88	kJ/mol	Joback Method
hf	1236.95	kJ/mol	Joback Method
hfus	85.20	kJ/mol	Joback Method
hvap	154.86	kJ/mol	Joback Method
log10ws	-21.96		Crippen Method
logp	14.401		Crippen Method
mcvol	466.680	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
tb	1637.22	K	Joback Method
tc	2017.91	K	Joback Method
tf	1222.36	K	Joback Method
vc	1.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2397.64	J/mol×K	1637.22	Joback Method
cpg	2598.70	J/mol×K	1700.67	Joback Method
cpg	2827.16	J/mol×K	1764.12	Joback Method
cpg	3085.18	J/mol×K	1827.56	Joback Method
cpg	3374.94	J/mol×K	1891.01	Joback Method
cpg	3698.62	J/mol×K	1954.46	Joback Method
cpg	4058.40	J/mol×K	2017.91	Joback Method
dvisc	0.3998904	Pa×s	1222.36	Joback Method

dvisc	0.3954435	Pa×s	1291.50	Joback Method
dvisc	0.3914907	Pa×s	1360.65	Joback Method
dvisc	0.3879543	Pa×s	1429.79	Joback Method
dvisc	0.3847717	Pa×s	1498.93	Joback Method
dvisc	0.3818926	Pa×s	1568.08	Joback Method
dvisc	0.3792756	Pa×s	1637.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72382924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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