Pyrene, 1,6-bis(1,1-dimethylethyl)-

Other names: 1,6-Di-tert-butylpyrene
Inchi: InChI=1S/C24H26/c1-23(2,3)19-13-9-15-8-12-18-20(24(4,5)6)14-10-16-7-11-17(19)21(15
InchiKey: OJKOMTHSAKFOHL-UHFFFAOYSA-N
Formula: C24H26
SMILES: CC(C)(C)c1ccc2ccc3c(C(C)(C)C)ccc4ccc1c2c43
Mol. weight [g/mol]: 314.46
CAS: 55044-29-6

Physical Properties

Property code	Value	Unit	Source
gf	544.96	kJ/mol	Joback Method
hf	162.21	kJ/mol	Joback Method
hfus	29.61	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.179		Crippen Method
mcvol	271.180	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
tb	837.90	K	Joback Method
tc	1081.18	K	Joback Method
tf	545.96	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.66	J/mol×K	837.90	Joback Method
cpg	901.63	J/mol×K	1040.63	Joback Method
cpg	885.19	J/mol×K	1000.09	Joback Method
cpg	868.82	J/mol×K	959.54	Joback Method
cpg	852.29	J/mol×K	918.99	Joback Method
cpg	835.32	J/mol×K	878.45	Joback Method
cpg	918.41	J/mol×K	1081.18	Joback Method
dvisc	0.0005561	Pa×s	837.90	Joback Method

dvisc	0.0006281	Pa×s	789.24	Joback Method
dvisc	0.0007210	Pa×s	740.59	Joback Method
dvisc	0.0008437	Pa×s	691.93	Joback Method
dvisc	0.0010112	Pa×s	643.27	Joback Method
dvisc	0.0012483	Pa×s	594.62	Joback Method
dvisc	0.0016000	Pa×s	545.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55044296&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