9-Tert-butyl-9,10-(dewar anthracene)

Inchi: InChI=1S/C18H18/c1-17(2,3)18-14-10-6-4-8-12(14)16(18)13-9-5-7-11-15(13)18/h4-11,16
InchiKey: ISMYYTMVFOAZIS-UHFFFAOYSA-N
Formula: C18H18
SMILES: CC(C)(C)C12c3ccccc3C1c1ccccc12
Mol. weight [g/mol]: 234.34
CAS: 76008-29-2

Physical Properties

Property code	Value	Unit	Source
gf	473.49	kJ/mol	Joback Method
hf	212.00	kJ/mol	Joback Method
hfus	20.64	kJ/mol	Joback Method
hvap	58.23	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.478		Crippen Method
mcvol	195.240	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
tb	667.97	K	Joback Method
tc	914.78	K	Joback Method
tf	446.78	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.05	J/mol×K	667.97	Joback Method
cpg	554.14	J/mol×K	709.11	Joback Method
cpg	570.16	J/mol×K	750.24	Joback Method
cpg	585.48	J/mol×K	791.38	Joback Method
cpg	600.48	J/mol×K	832.51	Joback Method
cpg	615.53	J/mol×K	873.65	Joback Method
cpg	631.00	J/mol×K	914.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76008292&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
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