Tribenzo[jk,qr,uv]naphtho[2,1,8,7-defg]pentacene

Inchi: InChI=1S/C36H18/c1-5-19-6-2-10-25-29(19)23(8-1)24-9-4-12-27-33(24)34(25)28-18-17-2
InchiKey: ZEKNUAHTJOBNED-UHFFFAOYSA-N
Formula: C36H18
SMILES: c1cc2cccc3c2c(c1)c1cccc2c1c3c1ccc3ccc4ccc5cccc6c5c4c3c1c62
Mol. weight [g/mol]: 450.53
CAS: 117726-82-6

Physical Properties

Property code	Value	Unit	Source
gf	1230.18	kJ/mol	Joback Method
hf	941.65	kJ/mol	Joback Method
hfus	62.03	kJ/mol	Joback Method
hvap	116.15	kJ/mol	Joback Method
log10ws	-15.96		Crippen Method
logp	10.379		Crippen Method
mcvol	332.100	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
tb	1237.32	K	Joback Method
tc	1526.05	K	Joback Method
tf	935.20	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.67	J/mol×K	1237.32	Joback Method
cpg	1213.56	J/mol×K	1285.44	Joback Method
cpg	1268.03	J/mol×K	1333.56	Joback Method
cpg	1329.84	J/mol×K	1381.68	Joback Method
cpg	1399.76	J/mol×K	1429.81	Joback Method
cpg	1478.54	J/mol×K	1477.93	Joback Method
cpg	1566.95	J/mol×K	1526.05	Joback Method
dvisc	0.1858032	Pa×s	935.20	Joback Method
dvisc	0.1893636	Pa×s	985.55	Joback Method

dvisc	0.1926365	Pa×s	1035.91	Joback Method
dvisc	0.1956549	Pa×s	1086.26	Joback Method
dvisc	0.1984470	Pa×s	1136.61	Joback Method
dvisc	0.2010371	Pa×s	1186.97	Joback Method
dvisc	0.2034462	Pa×s	1237.32	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=C117726826&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