Benzo[j]benzo[2,1-a!3,4-a']dianthracene

Other names: Benzo[j]benzo[2,1-a:3,4-a']dianthracene
Inchi: InChI=1S/C34H20/c1-2-7-25-19-31-27(17-24(25)6-1)15-12-22-10-11-23-13-16-28-18-26-
InchiKey: UFOJYKFBAGIOGQ-UHFFFAOYSA-N
Formula: C34H20
SMILES: c1ccc2cc3c(ccc4ccc5ccc6cc7ccc8ccccc8c7cc6c5c43)cc2c1
Mol. weight [g/mol]: 428.52
CAS: 122961-15-3

Physical Properties

Property code	Value	Unit	Source
gf	1036.58	kJ/mol	Joback Method
hf	760.11	kJ/mol	Joback Method
hfus	54.66	kJ/mol	Joback Method
hvap	109.01	kJ/mol	Joback Method
log10ws	-14.10		Crippen Method
logp	9.759		Crippen Method
mcvol	329.940	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
tb	1166.74	K	Joback Method
tc	1453.32	K	Joback Method
tf	803.38	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.53	J/mol×K	1166.74	Joback Method
cpg	1112.70	J/mol×K	1214.50	Joback Method
cpg	1143.78	J/mol×K	1262.27	Joback Method
cpg	1178.32	J/mol×K	1310.03	Joback Method
cpg	1216.88	J/mol×K	1357.79	Joback Method
cpg	1259.98	J/mol×K	1405.55	Joback Method
cpg	1308.19	J/mol×K	1453.32	Joback Method
dvisc	0.0069004	Pa×s	803.38	Joback Method

dvisc	0.0062390	Pa×s	863.94	Joback Method
dvisc	0.0057159	Pa×s	924.50	Joback Method
dvisc	0.0052934	Pa×s	985.06	Joback Method
dvisc	0.0049459	Pa×s	1045.62	Joback Method
dvisc	0.0046557	Pa×s	1106.18	Joback Method
dvisc	0.0044102	Pa×s	1166.74	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=C122961153&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