4H-Dibenzo[a,de]pentacene

Inchi: InChI=1S/C29H18/c1-2-7-19-13-23-16-27-24(15-22(23)12-18(19)6-1)17-28-25-10-4-3-8-2
InchiKey: BZZXPEWKRBRGLZ-UHFFFAOYSA-N
Formula: C29H18
SMILES: c1ccc2c(c1)Cc1cccc3c1c-2cc1cc2cc4ccccc4cc2cc13
Mol. weight [g/mol]: 366.45
CAS: 198-45-8

Physical Properties

Property code	Value	Unit	Source
gf	879.60	kJ/mol	Joback Method
hf	632.09	kJ/mol	Joback Method
hfus	45.95	kJ/mol	Joback Method
hvap	95.11	kJ/mol	Joback Method
log10ws	-11.64		Crippen Method
logp	7.871		Crippen Method
mcvol	283.250	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
tb	1024.95	K	Joback Method
tc	1300.68	K	Joback Method
tf	704.57	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.84	J/mol×K	1024.95	Joback Method
cpg	990.36	J/mol×K	1254.73	Joback Method
cpg	963.63	J/mol×K	1208.77	Joback Method
cpg	939.34	J/mol×K	1162.82	Joback Method
cpg	917.07	J/mol×K	1116.86	Joback Method
cpg	896.39	J/mol×K	1070.91	Joback Method
cpg	1019.99	J/mol×K	1300.68	Joback Method
dvisc	0.0041231	Pa×s	1024.95	Joback Method
dvisc	0.0043305	Pa×s	971.55	Joback Method

dvisc	0.0045744	Pa×s	918.16	Joback Method
dvisc	0.0048648	Pa×s	864.76	Joback Method
dvisc	0.0052157	Pa×s	811.36	Joback Method
dvisc	0.0056471	Pa×s	757.97	Joback Method
dvisc	0.0061882	Pa×s	704.57	Joback Method

Sources

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=C198458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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