

Tetrabenzo[de,jk,op,uv]pentacene

Inchi:	InChI=1S/C34H18/c1-5-19-13-14-20-6-2-10-24-28-18-30-26-12-4-8-22-16-15-21-7-3-11-2
InchiKey:	ZHRFYICOTBZCLJ-UHFFFAOYSA-N
Formula:	C34H18
SMILES:	<chem>c1cc2ccc3cccc4c5cc6c(cc5c(c1)c2c34)c1cccc2ccc3cccc6c3c21</chem>
Mol. weight [g/mol]:	426.51
CAS:	109587-17-9

Physical Properties

Property code	Value	Unit	Source
gf	1122.08	kJ/mol	Joback Method
hf	848.79	kJ/mol	Joback Method
hfus	57.24	kJ/mol	Joback Method
hvap	110.04	kJ/mol	Joback Method
log10ws	-14.74		Crippen Method
logp	9.788		Crippen Method
mcvol	319.080	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	1175.30	K	Joback Method
tc	1459.00	K	Joback Method
tf	861.16	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.65	J/molxK	1175.30	Joback Method
cpg	1288.31	J/molxK	1411.72	Joback Method
cpg	1231.96	J/molxK	1364.44	Joback Method
cpg	1181.95	J/molxK	1317.15	Joback Method
cpg	1137.66	J/molxK	1269.87	Joback Method
cpg	1098.44	J/molxK	1222.58	Joback Method
cpg	1351.65	J/molxK	1459.00	Joback Method
dvisc	0.0465239	Paxs	1175.30	Joback Method
dvisc	0.0467905	Paxs	1122.94	Joback Method

dvisc	0.0470849	Paxs	1070.59	Joback Method
dvisc	0.0474118	Paxs	1018.23	Joback Method
dvisc	0.0477768	Paxs	965.87	Joback Method
dvisc	0.0481869	Paxs	913.52	Joback Method
dvisc	0.0486510	Paxs	861.16	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=C109587179&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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