Tetrabenzo[c,m,pqr,tuv]picene

Inchi:	InChI=1S/C34H18/c1-3-7-23-19(5-1)17-21-9-11-27-28-12-10-22-18-20-6-2-4-8-24(20)26-
InchiKey:	FVVWCSNRORRPPI-UHFFFAOYSA-N
Formula:	C34H18
SMILES:	c1ccc2c(c1)cc1ccc3c4ccc5cc6ccccc6c6ccc(c7ccc2c1c37)c4c56
Mol. weight [g/mol]:	426.51
CAS:	188-87-4

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
ie	6.48 ± 0.02	eV	NIST Webbook
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	1351.65	J/mol×K	1459.00	Joback Method
cpg	1288.31	J/mol×K	1411.72	Joback Method
cpg	1231.96	J/mol×K	1364.44	Joback Method
cpg	1181.95	J/mol×K	1317.15	Joback Method
cpg	1137.66	J/mol×K	1269.87	Joback Method
cpg	1098.44	J/mol×K	1222.58	Joback Method
cpg	1063.65	J/mol×K	1175.30	Joback Method
dvisc	0.0486510	Pa×s	861.16	Joback Method

dvisc	0.0465239	Pa×s	1175.30	Joback Method
dvisc	0.0467905	Pa×s	1122.94	Joback Method
dvisc	0.0470849	Pa×s	1070.59	Joback Method
dvisc	0.0474118	Pa×s	1018.23	Joback Method
dvisc	0.0477768	Pa×s	965.87	Joback Method
dvisc	0.0481869	Pa×s	913.52	Joback Method
hsubt	195.80	kJ/mol	643.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C188874&Units=SI

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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