Dibenzo[m,pqr]naptho[1,2,3,4-tuv]picene

Inchi: InChI=1S/C34H18/c1-2-8-22-20(6-1)18-21-13-15-29-32-27(17-16-26(22)31(21)32)28-14-
InchiKey: AYMPPZHDKKQMLT-UHFFFAOYSA-N
Formula: C34H18
SMILES: c1ccc2c(c1)cc1ccc3c4c(ccc2c14)c1ccc2cccc4c5ccccc5c3c1c24
Mol. weight [g/mol]: 426.51
CAS: 190-93-2

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	6.59 ± 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	1063.65	J/mol×K	1175.30	Joback Method
cpg	1098.44	J/mol×K	1222.58	Joback Method
cpg	1137.66	J/mol×K	1269.87	Joback Method
cpg	1181.95	J/mol×K	1317.15	Joback Method
cpg	1231.96	J/mol×K	1364.44	Joback Method
cpg	1288.31	J/mol×K	1411.72	Joback Method
cpg	1351.65	J/mol×K	1459.00	Joback Method
dvisc	0.0486510	Pa×s	861.16	Joback Method

dvisc	0.0481869	Pa×s	913.52	Joback Method
dvisc	0.0477768	Pa×s	965.87	Joback Method
dvisc	0.0474118	Pa×s	1018.23	Joback Method
dvisc	0.0470849	Pa×s	1070.59	Joback Method
dvisc	0.0467905	Pa×s	1122.94	Joback Method
dvisc	0.0465239	Pa×s	1175.30	Joback Method
hsubt	154.10	kJ/mol	540.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C190932&Units=SI
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

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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