Naphthaceno[2,1,12,11-opqra]naphthacene

Inchi: InChI=1S/C30H16/c1-3-7-23-17(5-1)13-21-15-19-10-12-26-24-8-4-2-6-18(24)14-22-16-20
InchiKey: AHVOGQHPOOFLNU-UHFFFAOYSA-N
Formula: C30H16
SMILES: c1ccc2c(c1)cc1cc3ccc4c5ccccc5cc5cc6ccc2c1c6c3c54
Mol. weight [g/mol]: 376.45
CAS: 188-42-1

Physical Properties

Property code	Value	Unit	Source
gf	991.38	kJ/mol	Joback Method
hf	751.75	kJ/mol	Joback Method
hfus	50.25	kJ/mol	Joback Method
hvap	98.83	kJ/mol	Joback Method
ie	6.58	eV	NIST Webbook
ie	6.19	eV	NIST Webbook
log10ws	-12.93		Crippen Method
logp	8.635		Crippen Method
mcvol	282.180	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
tb	1059.82	K	Joback Method
tc	1334.83	K	Joback Method
tf	770.86	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.53	J/mol×K	1059.82	Joback Method
cpg	900.56	J/mol×K	1105.65	Joback Method
cpg	926.04	J/mol×K	1151.49	Joback Method
cpg	954.48	J/mol×K	1197.32	Joback Method
cpg	986.42	J/mol×K	1243.16	Joback Method
cpg	1022.37	J/mol×K	1288.99	Joback Method
cpg	1062.84	J/mol×K	1334.83	Joback Method

dvisc	0.0277526	Pa×s	770.86	Joback Method
dvisc	0.0275076	Pa×s	819.02	Joback Method
dvisc	0.0272917	Pa×s	867.18	Joback Method
dvisc	0.0270999	Pa×s	915.34	Joback Method
dvisc	0.0269285	Pa×s	963.50	Joback Method
dvisc	0.0267743	Pa×s	1011.66	Joback Method
dvisc	0.0266349	Pa×s	1059.82	Joback Method

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=C188421&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
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