

Benzo[pqr]naphtho[8,1,2-cde]picene

Inchi:	InChI=1S/C30H16/c1-3-17-7-9-21-15-26-24-14-12-20-6-2-4-18-8-10-22(30(24)28(18)20)
InchiKey:	NCECVMZBASVXIW-UHFFFAOYSA-N
Formula:	C30H16
SMILES:	<chem>c1cc2ccc3cc4c(cc5ccc6cccc7ccc4c5c67)c4ccc(c1)c2c34</chem>
Mol. weight [g/mol]:	376.45
CAS:	111728-58-6

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
log10ws	-12.93		Crippen Method
logp	8.635		Crippen Method
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.53	J/molxK	1059.82	Joback Method
cpg	1022.37	J/molxK	1288.99	Joback Method
cpg	986.42	J/molxK	1243.16	Joback Method
cpg	954.48	J/molxK	1197.32	Joback Method
cpg	926.04	J/molxK	1151.49	Joback Method
cpg	900.56	J/molxK	1105.65	Joback Method
cpg	1062.84	J/molxK	1334.83	Joback Method
dvisc	0.0266349	Paxs	1059.82	Joback Method
dvisc	0.0267743	Paxs	1011.66	Joback Method

dvisc	0.0269285	Paxs	963.50	Joback Method
dvisc	0.0270999	Paxs	915.34	Joback Method
dvisc	0.0272917	Paxs	867.18	Joback Method
dvisc	0.0275076	Paxs	819.02	Joback Method
dvisc	0.0277526	Paxs	770.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C111728586&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
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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