Benzo[pqr]naphtho[1,2-b]perylene

Inchi: InChI=1S/C30H16/c1-2-7-20-17(5-1)13-15-24-23-10-4-9-22-21-8-3-6-18-11-12-19-14-16-
InchiKey: OLERCWNZGJZODU-UHFFFAOYSA-N
Formula: C30H16
SMILES: c1ccc2c(c1)ccc1c3cccc4c5cccc6ccc7ccc(c21)c(c34)c7c65
Mol. weight [g/mol]: 376.45
CAS: 120835-57-6

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
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:	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=C120835576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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