BENZO[QR]NAPHTHO[2,1,8,7-FGHI]PENTACENE

Inchi: InChI=1S/C30H16/c1-2-7-19-18(6-1)16-26-23-11-5-10-22-20-8-3-4-9-21(20)25-15-13-17-
InchiKey: AVVLVJLIKRMPQZ-UHFFFAOYSA-N
Formula: C30H16
SMILES: c1ccc2c(c1)cc1c3cccc4c5ccccc5c5ccc6ccc2c1c6c5c43
Mol. weight [g/mol]: 376.46

Physical Properties

Property code	Value	Unit	Source
hf	519.75	kJ/mol	Cheméo Relay (1.0)
hfus	50.25	kJ/mol	Joback Method
hvap	182.60	kJ/mol	Cheméo Relay (1.0)
ie	7.27	eV	NIST Webbook
ie	7.03	eV	NIST Webbook
ie	6.97	eV	NIST Webbook
ie	6.97	eV	NIST Webbook
log10ws	-11.44		Cheméo Relay (1.0)
logp	8.635		Crippen Method
mcvol	282.180	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
tb	939.78	K	Cheméo Relay (1.0)
tc	1338.93	K	Cheméo Relay (1.0)
tf	568.78	K	Cheméo Relay (1.0)
vc	1.134	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C190874&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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