

Benzo[Imn]naphtho[2,1,8-qa]perylene

Inchi:	InChI=1S/C28H14/c1-3-15-9-11-19-13-20-12-10-17-8-7-16-4-2-6-21-22-14-18(5-1)23(15)
InchiKey:	CPOHOZKFLNGLFK-UHFFFAOYSA-N
Formula:	C28H14
SMILES:	<chem>c1cc2ccc3cc4ccc5ccc6cccc7c8cc(c1)c2c3c8c4c5c67</chem>
Mol. weight [g/mol]:	350.41
CAS:	75449-94-4

Physical Properties

Property code	Value	Unit	Source
gf	968.78	kJ/mol	Joback Method
hf	747.57	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	93.74	kJ/mol	Joback Method
log10ws	-12.35		Crippen Method
logp	8.072		Crippen Method
mcvol	258.300	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
tb	1006.36	K	Joback Method
tc	1275.89	K	Joback Method
tf	754.60	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.55	J/molxK	1006.36	Joback Method
cpg	797.63	J/molxK	1051.28	Joback Method
cpg	819.89	J/molxK	1096.20	Joback Method
cpg	844.84	J/molxK	1141.13	Joback Method
cpg	872.97	J/molxK	1186.05	Joback Method
cpg	904.81	J/molxK	1230.97	Joback Method
cpg	940.85	J/molxK	1275.89	Joback Method
dvisc	0.0530229	Paxs	754.60	Joback Method
dvisc	0.0545360	Paxs	796.56	Joback Method

dvisc	0.0559346	Paxs	838.52	Joback Method
dvisc	0.0572308	Paxs	880.48	Joback Method
dvisc	0.0584351	Paxs	922.44	Joback Method
dvisc	0.0595567	Paxs	964.40	Joback Method
dvisc	0.0606036	Paxs	1006.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75449944&Units=SI
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

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
mccvol:	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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