Pentalene

Inchi: InChI=1S/C8H6/c1-3-7-5-2-6-8(7)4-1/h1-6H
InchiKey: GUVXZFRDPCKWEM-UHFFFAOYSA-N
Formula: C8H6
SMILES: C1=CC2=CC=CC2=C1
Mol. weight [g/mol]: 102.13
CAS: 250-25-9

Physical Properties

Property code	Value	Unit	Source
gf	229.78	kJ/mol	Joback Method
hf	173.69	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	36.68	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.979		Crippen Method
mcvol	84.660	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
tb	420.40	K	Joback Method
tc	643.77	K	Joback Method
tf	245.32	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.98	J/mol×K	420.40	Joback Method
cpg	159.05	J/mol×K	457.63	Joback Method
cpg	169.17	J/mol×K	494.86	Joback Method
cpg	178.40	J/mol×K	532.09	Joback Method
cpg	186.82	J/mol×K	569.32	Joback Method
cpg	194.51	J/mol×K	606.55	Joback Method
cpg	201.54	J/mol×K	643.77	Joback Method
dvisc	0.0008643	Pa×s	245.32	Joback Method
dvisc	0.0007055	Pa×s	274.50	Joback Method

dvisc	0.0005988	Pa×s	303.68	Joback Method
dvisc	0.0005230	Pa×s	332.86	Joback Method
dvisc	0.0004669	Pa×s	362.04	Joback Method
dvisc	0.0004239	Pa×s	391.22	Joback Method
dvisc	0.0003901	Pa×s	420.40	Joback Method

Sources

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=C250259&Units=SI
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
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