9-n-propylphenanthrene

Other names: Phenanthrene, 9-propyl-
Inchi: InChI=1S/C17H16/c1-2-7-13-12-14-8-3-4-9-16(14)17-11-6-5-10-15(13)17/h3-6,8-12H,2,7
InchiKey: PIWHTUVAMGYSIC-UHFFFAOYSA-N
Formula: C17H16
SMILES: CCCc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]: 220.31
CAS: 17024-03-2

Physical Properties

Property code	Value	Unit	Source
gf	398.71	kJ/mol	Joback Method
hf	201.52	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.946		Crippen Method
mcvol	187.710	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	350.30		NIST Webbook
rinpol	350.30		NIST Webbook
rinpol	350.30		NIST Webbook
tb	662.96	K	Joback Method
tc	901.48	K	Joback Method
tf	398.21	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.25	J/mol×K	662.96	Joback Method
cpg	497.56	J/mol×K	702.71	Joback Method
cpg	512.69	J/mol×K	742.47	Joback Method
cpg	526.74	J/mol×K	782.22	Joback Method
cpg	539.84	J/mol×K	821.98	Joback Method

cpg	552.12	J/mol×K	861.73	Joback Method
cpg	563.71	J/mol×K	901.48	Joback Method
dvisc	0.0014293	Pa×s	398.21	Joback Method
dvisc	0.0010458	Pa×s	442.34	Joback Method
dvisc	0.0008099	Pa×s	486.46	Joback Method
dvisc	0.0006544	Pa×s	530.59	Joback Method
dvisc	0.0005463	Pa×s	574.71	Joback Method
dvisc	0.0004680	Pa×s	618.84	Joback Method
dvisc	0.0004093	Pa×s	662.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17024032&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume