

Phenanthrene, 9-nonyl-

Inchi:	InChI=1S/C23H28/c1-2-3-4-5-6-7-8-13-19-18-20-14-9-10-15-21(20)23-17-12-11-16-22(1
InchiKey:	ZCLFNENYAUUAFA-UHFFFAOYSA-N
Formula:	C23H28
SMILES:	CCCCCCCCc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]:	304.47
CAS:	16740-38-8

Physical Properties

Property code	Value	Unit	Source
gf	449.23	kJ/mol	Joback Method
hf	77.68	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	73.67	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	7.286		Crippen Method
mcvol	272.250	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
tb	800.24	K	Joback Method
tc	1016.49	K	Joback Method
tf	465.83	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.04	J/molxK	800.24	Joback Method
cpg	829.06	J/molxK	836.28	Joback Method
cpg	846.07	J/molxK	872.32	Joback Method
cpg	862.16	J/molxK	908.37	Joback Method
cpg	877.46	J/molxK	944.41	Joback Method
cpg	892.07	J/molxK	980.45	Joback Method
cpg	906.11	J/molxK	1016.49	Joback Method
dvisc	0.0012776	Paxs	465.83	Joback Method
dvisc	0.0008431	Paxs	521.57	Joback Method

dvisc	0.0006029	Paxs	577.30	Joback Method
dvisc	0.0004573	Paxs	633.04	Joback Method
dvisc	0.0003628	Paxs	688.77	Joback Method
dvisc	0.0002979	Paxs	744.50	Joback Method
dvisc	0.0002515	Paxs	800.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16740388&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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