

Phenanthrene, 1,2,7-trimethyl-

Inchi:	InChI=1S/C17H16/c1-11-4-7-16-14(10-11)6-9-15-13(3)12(2)5-8-17(15)16/h4-10H,1-3H3
InchiKey:	YAJODSBSLFRPN-UHFFFAOYSA-N
Formula:	C17H16
SMILES:	<chem>Cc1ccc2c(ccc3c(C)c(C)ccc32)c1</chem>
Mol. weight [g/mol]:	220.31
CAS:	60490-68-8

Physical Properties

Property code	Value	Unit	Source
gf	379.45	kJ/mol	Joback Method
hf	178.58	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	4.918		Crippen Method
mcvol	187.710	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
tb	672.92	K	Joback Method
tc	913.19	K	Joback Method
tf	423.25	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.54	J/molxK	672.92	Joback Method
cpg	549.32	J/molxK	873.15	Joback Method
cpg	537.11	J/molxK	833.10	Joback Method
cpg	524.14	J/molxK	793.06	Joback Method
cpg	510.29	J/molxK	753.01	Joback Method
cpg	495.46	J/molxK	712.97	Joback Method
cpg	560.86	J/molxK	913.19	Joback Method
dvisc	0.0004125	Paxs	672.92	Joback Method
dvisc	0.0004614	Paxs	631.31	Joback Method

dvisc	0.0005244	Paxs	589.70	Joback Method
dvisc	0.0006077	Paxs	548.09	Joback Method
dvisc	0.0007214	Paxs	506.47	Joback Method
dvisc	0.0008831	Paxs	464.86	Joback Method
dvisc	0.0011249	Paxs	423.25	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=C60490688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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