Phenanthrene, 9-bromo-

Other names:	9-Bromophenanthrene
	9-Phenanthryl bromide
	9-Phenathryl bromide
Inchi:	InChI=1S/C14H9Br/c15-14-9-10-5-1-2-6-11(10)12-7-3-4-8-13(12)14/h1-9H
InchiKey:	RSQXKVWKJVUZDG-UHFFFAOYSA-N
Formula:	C14H9Br
SMILES:	Brc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]:	257.12
CAS:	573-17-1

Physical Properties

Property code	Value	Unit	Source
gf	387.77	kJ/mol	Joback Method
hf	289.77	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	4.755		Crippen Method
mcvol	162.940	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	660.48	K	Joback Method
tc	927.78	K	Joback Method
tf	424.20	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.67	J/mol×K	660.48	Joback Method
cpg	380.45	J/mol×K	705.03	Joback Method
cpg	392.09	J/mol×K	749.58	Joback Method
cpg	402.76	J/mol×K	794.13	Joback Method
cpg	412.64	J/mol×K	838.68	Joback Method
cpg	421.90	J/mol×K	883.23	Joback Method

cpg	430.71	J/mol×K	927.78	Joback Method
dvisc	0.0014982	Pa×s	424.20	Joback Method
dvisc	0.0011666	Pa×s	463.58	Joback Method
dvisc	0.0009447	Pa×s	502.96	Joback Method
dvisc	0.0007888	Pa×s	542.34	Joback Method
dvisc	0.0006749	Pa×s	581.72	Joback Method
dvisc	0.0005890	Pa×s	621.10	Joback Method
dvisc	0.0005224	Pa×s	660.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	0.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C573171&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

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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume