

Phenanthrene-9,10-d2

Inchi:	InChI=1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-10H/i9D,10D
InchiKey:	YNPNZTXNASCQKK-QDRJLNDYSA-N
Formula:	C14H8D2
SMILES:	c1ccc2c(c1)ccc1ccccc12
Mol. weight [g/mol]:	180.24
CAS:	20722-48-9

Physical Properties

Property code	Value	Unit	Source
gf	383.08	kJ/mol	Joback Method
hf	274.91	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Joback Method
ie	8.03	eV	NIST Webbook
log10ws	-5.08		Crippen Method
logp	3.993		Crippen Method
mcvol	145.440	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	589.34	K	Joback Method
tc	843.18	K	Joback Method
tf	351.88	K	Joback Method
vc	0.555	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.16	J/molxK	589.34	Joback Method
cpg	396.94	J/molxK	800.87	Joback Method
cpg	386.47	J/molxK	758.56	Joback Method
cpg	375.10	J/molxK	716.26	Joback Method
cpg	362.69	J/molxK	673.95	Joback Method
cpg	349.09	J/molxK	631.65	Joback Method
cpg	406.65	J/molxK	843.18	Joback Method
dvisc	0.0004678	Paxs	589.34	Joback Method

dvisc	0.0005296	Paxs	549.76	Joback Method
dvisc	0.0006112	Paxs	510.19	Joback Method
dvisc	0.0007226	Paxs	470.61	Joback Method
dvisc	0.0008810	Paxs	431.03	Joback Method
dvisc	0.0011180	Paxs	391.46	Joback Method
dvisc	0.0014969	Paxs	351.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20722489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
ie:	Ionization energy
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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