Cd3-2-phenanthrene

Inchi: InChI=1S/C15H12/c1-11-6-9-15-13(10-11)8-7-12-4-2-3-5-14(12)15/h2-10H,1H3/i1D3
InchiKey: KANLOADZXMMCQA-FIBGUPNXSA-N
Formula: C15H12
SMILES: [2H]C([2H])([2H])c1ccc2c(ccc3ccccc32)c1
Mol. weight [g/mol]: 195.28

Physical Properties

Property code	Value	Unit	Source
af	0.5308		Cheméo Relay (1.0)
gf	381.87	kJ/mol	Joback Method
hf	-22.85	kJ/mol	Cheméo Relay (1.0)
hfus	21.91	kJ/mol	Joback Method
hvap	84.27	kJ/mol	Cheméo Relay (1.0)
ie	8.11	eV	Cheméo Relay (1.0)
log10ws	-6.03		Cheméo Relay (1.0)
logp	4.301		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	608.85	K	Cheméo Relay (1.0)
tc	1002.36	K	Cheméo Relay (1.0)
tf	408.21	K	Cheméo Relay (1.0)
vc	0.667	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.22	J/mol×K	617.20	Joback Method
cpg	456.90	J/mol×K	866.35	Joback Method
cpg	446.52	J/mol×K	824.83	Joback Method
cpg	435.41	J/mol×K	783.30	Joback Method
cpg	423.46	J/mol×K	741.78	Joback Method
cpg	410.54	J/mol×K	700.25	Joback Method
cpg	396.50	J/mol×K	658.73	Joback Method
dvisc	0.0006946	Pa×s	496.44	Joback Method

dvisc	0.0004577	Pa×s	617.20	Joback Method
dvisc	0.0005158	Pa×s	576.95	Joback Method
dvisc	0.0005920	Pa×s	536.69	Joback Method
dvisc	0.0013787	Pa×s	375.67	Joback Method
dvisc	0.0008385	Pa×s	456.18	Joback Method
dvisc	0.0010496	Pa×s	415.93	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004217&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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