Perhydropyrene, # 4

Other names:	Perhydropyrene, # 5
	Perhydropyrene, # 6
	Perhydropyrene, # 7
	Perhydropyrene, # 1
	Perhydropyrene, # 2
	Perhydropyrene, # 3
	Perhydropyrene, # 8
	Perhydropyrene, # 9
	Perhydropyrene
Inchi:	InChI=1S/C16H26/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h11-16H,1-10H2
InchiKey:	BYBPEZLZCGOWIS-UHFFFAOYSA-N
Formula:	C16H26
SMILES:	C1CC2CCC3CCCC4CCC(C1)C2C34
Mol. weight [g/mol]:	218.38
CAS:	16291-77-3

Physical Properties

Property code	Value	Unit	Source
gf	263.02	kJ/mol	Joback Method
hf	-147.69	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	50.93	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
log10ws	-4.65		Crippen Method
logp	4.639		Crippen Method
mcvol	192.860	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1767.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1750.00		NIST Webbook
tb	600.18	K	Joback Method
tc	832.27	K	Joback Method
tf	319.28	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.83	J/mol×K	600.18	Joback Method
cpg	693.41	J/mol×K	793.58	Joback Method
cpg	672.51	J/mol×K	754.90	Joback Method
cpg	650.04	J/mol×K	716.22	Joback Method
cpg	625.86	J/mol×K	677.54	Joback Method
cpg	599.84	J/mol×K	638.86	Joback Method
cpg	712.88	J/mol×K	832.27	Joback Method
dvisc	0.0022349	Pa×s	600.18	Joback Method
dvisc	0.0022704	Pa×s	553.36	Joback Method
dvisc	0.0023131	Pa×s	506.55	Joback Method
dvisc	0.0023657	Pa×s	459.73	Joback Method
dvisc	0.0024318	Pa×s	412.91	Joback Method
dvisc	0.0025174	Pa×s	366.10	Joback Method
dvisc	0.0026326	Pa×s	319.28	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16291773&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume