

6H-Pyrene, 2,3-dihydro-2,4-dimethyl

Inchi:	InChI=1S/C7H12O/c1-6-3-4-8-7(2)5-6/h3,7H,4-5H2,1-2H3
InchiKey:	ZBIMOHPRBACTOE-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CC1=CCOC(C)C1
Mol. weight [g/mol]:	112.17

Physical Properties

Property code	Value	Unit	Source
gf	-33.28	kJ/mol	Joback Method
hf	-219.18	kJ/mol	Joback Method
hfus	14.53	kJ/mol	Joback Method
hvap	37.07	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.742		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	818.00		NIST Webbook
tb	410.20	K	Joback Method
tc	616.97	K	Joback Method
tf	215.88	K	Joback Method
vc	0.367	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.82	J/molxK	410.20	Joback Method
cpg	205.84	J/molxK	444.66	Joback Method
cpg	219.21	J/molxK	479.12	Joback Method
cpg	231.93	J/molxK	513.58	Joback Method
cpg	244.03	J/molxK	548.05	Joback Method
cpg	255.52	J/molxK	582.51	Joback Method
cpg	266.40	J/molxK	616.97	Joback Method
dvisc	0.0038057	Paxs	215.88	Joback Method
dvisc	0.0018725	Paxs	248.27	Joback Method

dvisc	0.0010852	Paxs	280.65	Joback Method
dvisc	0.0007040	Paxs	313.04	Joback Method
dvisc	0.0004954	Paxs	345.43	Joback Method
dvisc	0.0003702	Paxs	377.81	Joback Method
dvisc	0.0002897	Paxs	410.20	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=R128159&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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