1-Methylacenaphthylene

Other names: Acenaphthylene, 1-methyl
Inchi: InChI=1S/C13H10/c1-9-8-11-6-2-4-10-5-3-7-12(9)13(10)11/h2-8H,1H3
InchiKey: QALUZRZBRMSBPM-UHFFFAOYSA-N
Formula: C13H10
SMILES: CC1=Cc2cccc3cccc1c23
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	359.27	kJ/mol	Joback Method
hf	238.62	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	50.78	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.714		Crippen Method
mcvol	135.650	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	266.57		NIST Webbook
rinpol	266.57		NIST Webbook
rinpol	265.24		NIST Webbook
tb	563.74	K	Joback Method
tc	803.57	K	Joback Method
tf	359.41	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.82	J/mol×K	563.74	Joback Method
cpg	319.14	J/mol×K	603.71	Joback Method
cpg	331.34	J/mol×K	643.68	Joback Method
cpg	342.56	J/mol×K	683.65	Joback Method
cpg	352.92	J/mol×K	723.63	Joback Method
cpg	362.55	J/mol×K	763.60	Joback Method

cpg	371.58	J/mol×K	803.57	Joback Method
dvisc	0.0012797	Pa×s	359.41	Joback Method
dvisc	0.0011239	Pa×s	393.47	Joback Method
dvisc	0.0010076	Pa×s	427.52	Joback Method
dvisc	0.0009181	Pa×s	461.58	Joback Method
dvisc	0.0008472	Pa×s	495.63	Joback Method
dvisc	0.0007900	Pa×s	529.69	Joback Method
dvisc	0.0007429	Pa×s	563.74	Joback Method

Sources

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=R15379&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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