Azulene,1-methyl-

Other names: 1-Methylazulene
Inchi: InChI=1S/C11H10/c1-9-7-8-10-5-3-2-4-6-11(9)10/h2-8H,1H3
InchiKey: WSQIUQGZWDQMEL-UHFFFAOYSA-N
Formula: C11H10
SMILES: Cc1ccc2cccccc1-2
Mol. weight [g/mol]: 142.20
CAS: 769-31-3

Physical Properties

Property code	Value	Unit	Source
gf	251.17	kJ/mol	Joback Method
hf	145.76	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	44.66	kJ/mol	Joback Method
ie	7.26 ± 0.03	eV	NIST Webbook
log10ws	-3.97		Crippen Method
logp	3.100		Crippen Method
mcvol	122.630	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1401.00		NIST Webbook
rinpol	1401.00		NIST Webbook
tb	501.72	K	Joback Method
tc	736.41	K	Joback Method
tf	285.37	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.16	J/mol×K	501.72	Joback Method
cpg	266.51	J/mol×K	540.83	Joback Method
cpg	279.78	J/mol×K	579.95	Joback Method
cpg	292.07	J/mol×K	619.06	Joback Method
cpg	303.43	J/mol×K	658.18	Joback Method

cpg	313.94	J/mol×K	697.29	Joback Method
cpg	323.67	J/mol×K	736.41	Joback Method
dvisc	0.0014596	Pa×s	285.37	Joback Method
dvisc	0.0009733	Pa×s	321.43	Joback Method
dvisc	0.0007043	Pa×s	357.49	Joback Method
dvisc	0.0005408	Pa×s	393.55	Joback Method
dvisc	0.0004341	Pa×s	429.60	Joback Method
dvisc	0.0003605	Pa×s	465.66	Joback Method
dvisc	0.0003074	Pa×s	501.72	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=C769313&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
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

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