

Azulene,5-methyl-

Other names:	5-Methylazulene
Inchi:	InChI=1S/C11H10/c1-9-4-2-5-10-6-3-7-11(10)8-9/h2-8H,1H3
InchiKey:	RGZLGZNMQMWYIM-UHFFFAOYSA-N
Formula:	C11H10
SMILES:	Cc1cccc2cccc-2c1
Mol. weight [g/mol]:	142.20
CAS:	1654-55-3

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	7.30 ± 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	1400.00		NIST Webbook
rinpol	1400.00		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/molxK	501.72	Joback Method
cpg	266.51	J/molxK	540.83	Joback Method
cpg	279.78	J/molxK	579.95	Joback Method
cpg	292.07	J/molxK	619.06	Joback Method
cpg	303.43	J/molxK	658.18	Joback Method

cpg	313.94	J/molxK	697.29	Joback Method
cpg	323.67	J/molxK	736.41	Joback Method
dvisc	0.0014596	Paxs	285.37	Joback Method
dvisc	0.0009733	Paxs	321.43	Joback Method
dvisc	0.0007043	Paxs	357.49	Joback Method
dvisc	0.0005408	Paxs	393.55	Joback Method
dvisc	0.0004341	Paxs	429.60	Joback Method
dvisc	0.0003605	Paxs	465.66	Joback Method
dvisc	0.0003074	Paxs	501.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1654553&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

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