1,4-Dimethylazulene

Inchi: InChI=1S/C12H12/c1-9-5-3-4-6-11-10(2)7-8-12(9)11/h3-8H,1-2H3
InchiKey: FKBGSRCZHMNHGG-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1ccc2c(C)ccccc1-2
Mol. weight [g/mol]: 156.22
CAS: 1127-69-1

Physical Properties

Property code	Value	Unit	Source
gf	249.96	kJ/mol	Joback Method
hf	113.65	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.408		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1555.20		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1528.00		NIST Webbook
ripol	2291.00		NIST Webbook
ripol	2291.00		NIST Webbook
tb	529.58	K	Joback Method
tc	761.14	K	Joback Method
tf	309.16	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.31	J/mol×K	529.58	Joback Method
cpg	361.06	J/mol×K	722.55	Joback Method

cpg	349.89	J/mol×K	683.95	Joback Method
cpg	337.89	J/mol×K	645.36	Joback Method
cpg	325.00	J/mol×K	606.77	Joback Method
cpg	311.16	J/mol×K	568.17	Joback Method
cpg	371.48	J/mol×K	761.14	Joback Method
dvisc	0.0002960	Pa×s	529.58	Joback Method
dvisc	0.0003443	Pa×s	492.84	Joback Method
dvisc	0.0004103	Pa×s	456.11	Joback Method
dvisc	0.0005043	Pa×s	419.37	Joback Method
dvisc	0.0006448	Pa×s	382.63	Joback Method
dvisc	0.0008686	Pa×s	345.90	Joback Method
dvisc	0.0012561	Pa×s	309.16	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1127691&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume