(+)-1,2,3,6-Tetrahydro-1,4-dimethylazulene

Inchi: InChI=1S/C12H16/c1-9-5-3-4-6-11-10(2)7-8-12(9)11/h4-6,10H,3,7-8H2,1-2H3
InchiKey: QOXYDBYDOMCGHM-UHFFFAOYSA-N
Formula: C12H16
SMILES: CC1=CCC=CC2=C1CCC2C
Mol. weight [g/mol]: 160.26

Physical Properties

Property code	Value	Unit	Source
gf	191.96	kJ/mol	Joback Method
hf	-10.78	kJ/mol	Joback Method
hfus	16.13	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.619		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
tb	521.61	K	Joback Method
tc	747.23	K	Joback Method
tf	290.88	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.07	J/mol×K	521.61	Joback Method
cpg	351.33	J/mol×K	559.21	Joback Method
cpg	368.45	J/mol×K	596.82	Joback Method
cpg	384.49	J/mol×K	634.42	Joback Method
cpg	399.49	J/mol×K	672.02	Joback Method
cpg	413.53	J/mol×K	709.63	Joback Method
cpg	426.65	J/mol×K	747.23	Joback Method

dvisc	0.0016585	Pa×s	290.88	Joback Method
dvisc	0.0010799	Pa×s	329.33	Joback Method
dvisc	0.0007692	Pa×s	367.79	Joback Method
dvisc	0.0005842	Pa×s	406.25	Joback Method
dvisc	0.0004653	Pa×s	444.70	Joback Method
dvisc	0.0003843	Pa×s	483.16	Joback Method
dvisc	0.0003265	Pa×s	521.61	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=R515667&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