cis-Salvene

Inchi: InChI=1S/C9H16/c1-5-6-7-9(4)8(2)3/h5-6,8H,4,7H2,1-3H3/b6-5-
InchiKey: KKKHJDOOIQCWIL-WAYWQWQTSA-N
Formula: C9H16
SMILES: C=C(CC=CC)C(C)C
Mol. weight [g/mol]: 124.22

Physical Properties

Property code	Value	Unit	Source
gf	181.97	kJ/mol	Joback Method
hf	-1.51	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	34.61	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.165		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	852.00		NIST Webbook
rinpol	852.00		NIST Webbook
tb	405.60	K	Joback Method
tc	587.83	K	Joback Method
tf	155.39	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.59	J/mol×K	405.60	Joback Method
cpg	256.69	J/mol×K	435.97	Joback Method
cpg	270.12	J/mol×K	466.34	Joback Method
cpg	282.90	J/mol×K	496.71	Joback Method
cpg	295.05	J/mol×K	527.08	Joback Method
cpg	306.62	J/mol×K	557.46	Joback Method
cpg	317.61	J/mol×K	587.83	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=R630989&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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