(Z)-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	859.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	863.00		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=R642229&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