geranial dimethyl acetal

Inchi: InChI=1S/C12H22O2/c1-10(2)7-6-8-11(3)9-12(13-4)14-5/h7,9,12H,6,8H2,1-5H3/b11-9+
InchiKey: ZSKAJFSSXURRGL-PKNBQFBNSA-N
Formula: C12H22O2
SMILES: COC(C=C(C)CCC=C(C)C)OC
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-18.94	kJ/mol	Joback Method
hf	-345.87	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	46.81	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.298		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1322.60		NIST Webbook
tb	526.44	K	Joback Method
tc	710.27	K	Joback Method
tf	216.38	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.35	J/mol×K	526.44	Joback Method
cpg	445.83	J/mol×K	557.08	Joback Method
cpg	461.59	J/mol×K	587.72	Joback Method
cpg	476.65	J/mol×K	618.36	Joback Method
cpg	491.03	J/mol×K	648.99	Joback Method
cpg	504.77	J/mol×K	679.63	Joback Method
cpg	517.86	J/mol×K	710.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R185612&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
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