

trans-Isogeraniol

Other names:	(E)-iso-geraniol
Inchi:	InChI=1S/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5-6,11H,4,7-8H2,1-3H3/b10-6+
InchiKey:	DTHIOPUFUOMHAY-UXBLZVDNSA-N
Formula:	C10H18O
SMILES:	CC(C)=CCC=C(C)CCO
Mol. weight [g/mol]:	154.25

Physical Properties

Property code	Value	Unit	Source
gf	39.84	kJ/mol	Joback Method
hf	-187.10	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	54.61	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.671		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
ripol	1812.00		NIST Webbook
tb	528.46	K	Joback Method
tc	705.46	K	Joback Method
tf	225.20	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.44	J/mol×K	528.46	Joback Method
cpg	357.23	J/mol×K	557.96	Joback Method
cpg	369.40	J/mol×K	587.46	Joback Method
cpg	380.97	J/mol×K	616.96	Joback Method
cpg	391.97	J/mol×K	646.46	Joback Method
cpg	402.45	J/mol×K	675.96	Joback Method
cpg	412.43	J/mol×K	705.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R295011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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