

geranial propylene glycol acetal (isomer)

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H22O2/c1-10(2)6-5-7-11(3)8-13-14-9-12(4)15-13/h6,8,12-13H,5,7,9H2,1-4

DWZRENGNFQNWQZ-DHZHZOJOSA-N

C13H22O2

CC(C)=CCCC(C)=CC1OCC(C)O1

210.31

Physical Properties

Property code	Value	Unit	Source
gf	58.52	kJ/mol	Joback Method
hf	-320.65	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	53.58	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.440		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
ripol	1884.00		NIST Webbook
ripol	1897.00		NIST Webbook
ripol	1884.00		NIST Webbook
tb	569.43	K	Joback Method
tc	774.18	K	Joback Method
tf	257.99	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.81	J/mol×K	569.43	Joback Method
cpg	499.11	J/mol×K	603.56	Joback Method
cpg	517.32	J/mol×K	637.68	Joback Method
cpg	534.48	J/mol×K	671.81	Joback Method
cpg	550.66	J/mol×K	705.93	Joback Method
cpg	565.90	J/mol×K	740.06	Joback Method
cpg	580.26	J/mol×K	774.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R441635&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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