

«alpha»-Cyclogeraniol acetate

Other names:	cyclogeraniol acetate
Inchi:	InChI=1S/C12H20O2/c1-9-6-5-7-12(3,4)11(9)8-14-10(2)13/h6,11H,5,7-8H2,1-4H3
InchiKey:	OGVKVTLZVLENPM-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OCC1C(C)=CCCC1(C)C
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
gf	-152.18	kJ/mol	Joback Method
hf	-440.28	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.932		Crippen Method
mvol	172.220	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
tb	569.51	K	Joback Method
tc	779.44	K	Joback Method
tf	337.48	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.86	J/molxK	569.51	Joback Method
cpg	452.86	J/molxK	604.50	Joback Method
cpg	469.91	J/molxK	639.49	Joback Method
cpg	486.10	J/molxK	674.48	Joback Method
cpg	501.52	J/molxK	709.46	Joback Method
cpg	516.24	J/molxK	744.45	Joback Method
cpg	530.36	J/molxK	779.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U158301&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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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