«beta»-Cyclogeraniol

Other names: 2,6,6-trimethylcyclohexene-1-methanol
Inchi: InChI=1S/C10H18O/c1-8-5-4-6-10(2,3)9(8)7-11/h11H,4-7H2,1-3H3
InchiKey: QWNGCDQJLXENDZ-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1=C(CO)C(C)(C)CCC1
Mol. weight [g/mol]: 154.25
CAS: 472-20-8

Physical Properties

Property code	Value	Unit	Source
gf	-73.84	kJ/mol	Joback Method
hf	-297.56	kJ/mol	Joback Method
hfus	11.72	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.505		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	1213.00		NIST Webbook
tb	549.29	K	Joback Method
tc	746.40	K	Joback Method
tf	320.36	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.72	J/mol×K	549.29	Joback Method
cpg	364.18	J/mol×K	582.14	Joback Method
cpg	377.88	J/mol×K	614.99	Joback Method
cpg	390.89	J/mol×K	647.84	Joback Method
cpg	403.30	J/mol×K	680.69	Joback Method
cpg	415.19	J/mol×K	713.55	Joback Method
cpg	426.64	J/mol×K	746.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C472208&Units=SI

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