2-Cyclohexen-1-ol, 3-(1-buten-1-yl), 2,4,4-trimethyl

Other names: 3-(but-1-enyl)-2,4,4-trimethylcyclohex-2-en-1-ol
Inchi: InChI=1S/C13H22O/c1-5-6-7-11-10(2)12(14)8-9-13(11,3)4/h6-7,12,14H,5,8-9H2,1-4H3/b
InchiKey: SPJJJLMGNIWHRG-VOTSOKGWSA-N
Formula: C13H22O
SMILES: CCC=CC1=C(C)C(O)CCC1(C)C
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	23.93	kJ/mol	Joback Method
hf	-262.60	kJ/mol	Joback Method
hfus	20.77	kJ/mol	Joback Method
hvap	61.75	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.450		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1337.00		NIST Webbook
tb	617.42	K	Joback Method
tc	814.43	K	Joback Method
tf	344.85	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.74	J/mol×K	617.42	Joback Method
cpg	496.04	J/mol×K	650.26	Joback Method
cpg	511.57	J/mol×K	683.09	Joback Method
cpg	526.41	J/mol×K	715.93	Joback Method
cpg	540.65	J/mol×K	748.76	Joback Method
cpg	554.39	J/mol×K	781.60	Joback Method
cpg	567.72	J/mol×K	814.43	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=R66059&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