3-(but-1-enyl)-2,4,4-trimethylcyclohexan-1-ol

Inchi: InChI=1S/C13H24O/c1-5-6-7-11-10(2)12(14)8-9-13(11,3)4/h6-7,10-12,14H,5,8-9H2,1-4H
InchiKey: ORUJVSLPJOWGCM-VOTSOKGWSA-N
Formula: C13H24O
SMILES: CCC=CC1C(C)C(O)CCC1(C)C
Mol. weight [g/mol]: 196.33

Physical Properties

Property code	Value	Unit	Source
gf	-2.19	kJ/mol	Joback Method
hf	-338.12	kJ/mol	Joback Method
hfus	22.47	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.386		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1342.00		NIST Webbook
tb	598.96	K	Joback Method
tc	792.23	K	Joback Method
tf	310.57	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.53	J/mol×K	598.96	Joback Method
cpg	522.11	J/mol×K	631.17	Joback Method
cpg	539.78	J/mol×K	663.38	Joback Method
cpg	556.60	J/mol×K	695.59	Joback Method
cpg	572.68	J/mol×K	727.81	Joback Method
cpg	588.10	J/mol×K	760.02	Joback Method
cpg	602.94	J/mol×K	792.23	Joback Method

Sources

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=R407066&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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