2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-bu

Other names: 2-Ethyl-4-(2,2,3-trimethylcyclopent-3-en-1-yl)but-2-en-1-ol
Inchi: InChI=1S/C14H24O/c1-5-12(10-15)7-9-13-8-6-11(2)14(13,3)4/h6-7,13,15H,5,8-10H2,1-4
InchiKey: KHQDWCKZXLWDNM-KPKJPENVSA-N
Formula: C14H24O
SMILES: CCC(=CCC1CC=C(C)C1(C)C)CO
Mol. weight [g/mol]: 208.34
CAS: 28219-61-6

Physical Properties

Property code	Value	Unit	Source
gf	45.53	kJ/mol	Joback Method
hf	-275.40	kJ/mol	Joback Method
hfus	24.54	kJ/mol	Joback Method
hvap	63.23	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.698		Crippen Method
mcvol	194.530	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1558.60		NIST Webbook
rinpol	1558.60		NIST Webbook
tb	630.93	K	Joback Method
tc	821.94	K	Joback Method
tf	333.16	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.72	J/mol×K	630.93	Joback Method
cpg	546.17	J/mol×K	662.76	Joback Method
cpg	561.85	J/mol×K	694.60	Joback Method
cpg	576.86	J/mol×K	726.43	Joback Method
cpg	591.30	J/mol×K	758.27	Joback Method
cpg	605.26	J/mol×K	790.10	Joback Method

cpg	618.84	J/mol×K	821.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28219616&Units=SI
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

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