Dihydro-«beta»-ionene

Inchi: InChI=1S/C13H22/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h5H,1,6-10H2,2-4H3
InchiKey: KQKAQIOEBKPBEA-UHFFFAOYSA-N
Formula: C13H22
SMILES: C=CCCC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 178.31

Physical Properties

Property code	Value	Unit	Source
gf	176.08	kJ/mol	Joback Method
hf	-81.82	kJ/mol	Joback Method
hfus	14.13	kJ/mol	Joback Method
hvap	44.76	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.479		Crippen Method
mcvol	174.570	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1424.00		NIST Webbook
tb	522.43	K	Joback Method
tc	728.30	K	Joback Method
tf	291.59	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.61	J/mol×K	522.43	Joback Method
cpg	429.88	J/mol×K	556.74	Joback Method
cpg	448.04	J/mol×K	591.05	Joback Method
cpg	465.21	J/mol×K	625.36	Joback Method
cpg	481.48	J/mol×K	659.68	Joback Method
cpg	496.96	J/mol×K	693.99	Joback Method
cpg	511.75	J/mol×K	728.30	Joback Method

Sources

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=R228987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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