(E)-Isovalencenal [eremophila-1(10),7(11)-dien-12-al

Inchi: InChI=1S/C15H22O/c1-11(10-16)13-7-8-14-6-4-5-12(2)15(14,3)9-13/h6,10,12H,4-5,7-9H

InchiKey: SVFQWLHYXVFRHQ-NVXNZCMISA-N

Formula: C15H22O

SMILES: CC(C=O)=C1CCC2=CCCC(C)C2(C)C1

Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	100.75	kJ/mol	Joback Method
hf	-189.76	kJ/mol	Joback Method
hfus	18.31	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	632.72	K	Joback Method
tc	861.77	K	Joback Method
tf	356.19	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.12	J/mol×K	632.72	Joback Method
cpg	547.19	J/mol×K	670.90	Joback Method
cpg	566.08	J/mol×K	709.07	Joback Method
cpg	583.95	J/mol×K	747.25	Joback Method
cpg	600.97	J/mol×K	785.42	Joback Method
cpg	617.33	J/mol×K	823.60	Joback Method
cpg	633.20	J/mol×K	861.77	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=R397890&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

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