(Z)-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/h7,10-11,14H,2,4-6
InchiKey: NRWGBVWLFAHFHR-PJYWTSEFSA-N
Formula: C15H22O
SMILES: C=C1CCCC2CC=C(C(C)C=O)CC12C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	114.48	kJ/mol	Joback Method
hf	-177.04	kJ/mol	Joback Method
hfus	14.62	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	624.92	K	Joback Method
tc	849.89	K	Joback Method
tf	358.47	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.34	J/mol×K	624.92	Joback Method
cpg	546.45	J/mol×K	662.41	Joback Method
cpg	565.35	J/mol×K	699.91	Joback Method
cpg	583.21	J/mol×K	737.40	Joback Method
cpg	600.19	J/mol×K	774.90	Joback Method
cpg	616.43	J/mol×K	812.39	Joback Method
cpg	632.10	J/mol×K	849.89	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=R199349&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