(E)-Eremophila-1(10),7(11)-dien-12-yl acetate

Inchi: InChI=1S/C17H26O2/c1-12(11-19-14(3)18)15-8-9-16-7-5-6-13(2)17(16,4)10-15/h7,13H,5
InchiKey: PAGIZIHMWSSCEF-NTCAYCPXSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC(C)=C1CCC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]: 262.39
CAS: 352461-71-3

Physical Properties

Property code	Value	Unit	Source
gf	-16.81	kJ/mol	Joback Method
hf	-390.26	kJ/mol	Joback Method
hfus	23.99	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.412		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1861.40		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1861.40		NIST Webbook
ripol	2422.00		NIST Webbook
ripol	2422.00		NIST Webbook
tb	706.11	K	Joback Method
tc	928.60	K	Joback Method
tf	408.89	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.65	J/mol×K	706.11	Joback Method
cpg	686.23	J/mol×K	743.19	Joback Method
cpg	705.80	J/mol×K	780.27	Joback Method

cpg	724.52	J/mol×K	817.36	Joback Method
cpg	742.53	J/mol×K	854.44	Joback Method
cpg	759.98	J/mol×K	891.52	Joback Method
cpg	777.02	J/mol×K	928.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C352461713&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume