(E)-2-((8R,8aS)-8,8a-Dimethyl-3,4,6,7,8,8a-hexahyd formate

Other names: Isovalencenyl formate
(E)-Eremophila-1(10),7(11)-dien-12-yl formate

Inchi: InChI=1S/C16H24O2/c1-12(10-18-11-17)14-7-8-15-6-4-5-13(2)16(15,3)9-14/h6,11,13H,4

InchiKey: SAHHFGUGGFKBSR-WYMLVPIESA-N

Formula: C16H24O2

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

Mol. weight [g/mol]: 248.36

CAS: 352457-47-7

Physical Properties

Property code	Value	Unit	Source
gf	4.17	kJ/mol	Joback Method
hf	-342.62	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	61.52	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.022		Crippen Method
mcvol	213.420	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	678.02	K	Joback Method
tc	899.88	K	Joback Method
tf	389.69	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.60	J/mol×K	678.02	Joback Method
cpg	629.50	J/mol×K	715.00	Joback Method
cpg	648.36	J/mol×K	751.97	Joback Method
cpg	666.35	J/mol×K	788.95	Joback Method
cpg	683.61	J/mol×K	825.93	Joback Method

cpg	700.28	J/mol×K	862.91	Joback Method
cpg	716.51	J/mol×K	899.88	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=C352457477&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