Formic acid, 3,7,11-trimethyl-1,6,10-dodecatrien-3-yl ester

Inchi: InChI=1S/C16H26O2/c1-6-16(5,18-13-17)12-8-11-15(4)10-7-9-14(2)3/h6,9,11,13H,1,7-8,

InchiKey: GJPVEZJRYIBIOD-RVDMUPIBSA-N

Formula: C16H26O2

SMILES: C=CC(C)(CCC=C(C)CCC=C(C)C)OC=O

Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	113.34	kJ/mol	Joback Method
hf	-259.83	kJ/mol	Joback Method
hfus	29.76	kJ/mol	Joback Method
hvap	58.45	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.577		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	638.09	K	Joback Method
tc	828.39	K	Joback Method
tf	296.89	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.21	J/mol×K	638.09	Joback Method
cpg	630.52	J/mol×K	669.81	Joback Method
cpg	646.88	J/mol×K	701.52	Joback Method
cpg	662.35	J/mol×K	733.24	Joback Method
cpg	676.98	J/mol×K	764.95	Joback Method
cpg	690.85	J/mol×K	796.67	Joback Method
cpg	703.99	J/mol×K	828.39	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=U132110&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