trans-Eudesma-4(15),7-dien-12-yl formate

Inchi: InChI=1S/C16H24O2/c1-12-5-4-7-16(3)8-6-14(9-15(12)16)13(2)10-18-11-17/h6,11,13,15
InchiKey: UZYFBQUUFYMFQV-AVVWSFFYSA-N
Formula: C16H24O2
SMILES: C=C1CCCC2(C)CC=C(C(C)COC=O)CC12
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	17.90	kJ/mol	Joback Method
hf	-329.90	kJ/mol	Joback Method
hfus	18.40	kJ/mol	Joback Method
hvap	60.43	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.878		Crippen Method
mcvol	213.420	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1745.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2330.00		NIST Webbook
tb	670.22	K	Joback Method
tc	888.41	K	Joback Method
tf	391.97	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.89	J/mol×K	670.22	Joback Method
cpg	628.79	J/mol×K	706.58	Joback Method
cpg	647.64	J/mol×K	742.95	Joback Method
cpg	665.58	J/mol×K	779.31	Joback Method
cpg	682.73	J/mol×K	815.68	Joback Method
cpg	699.23	J/mol×K	852.04	Joback Method
cpg	715.19	J/mol×K	888.41	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=R199329&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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