7-Oxodehydroabietic acid, methyl ester

Other names: Methyl 7-oxo-8,11,13-Abietatrien-18-oate
Inchi: InChI=1S/C21H28O3/c1-13(2)14-7-8-16-15(11-14)17(22)12-18-20(16,3)9-6-10-21(18,4)1
InchiKey: URPBIQPJABGDJD-UHFFFAOYSA-N
Formula: C21H28O3
SMILES: COC(=O)C1(C)CCCC2(C)c3ccc(C(C)C)cc3C(=O)CC12
Mol. weight [g/mol]: 328.45
CAS: 110936-78-2

Physical Properties

Property code	Value	Unit	Source
gf	-61.25	kJ/mol	Joback Method
hf	-507.54	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	76.51	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.634		Crippen Method
mcvol	270.280	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	878.02	K	Joback Method
tc	1121.58	K	Joback Method
tf	575.67	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.94	J/mol×K	878.02	Joback Method
cpg	920.89	J/mol×K	918.61	Joback Method
cpg	944.99	J/mol×K	959.21	Joback Method
cpg	969.55	J/mol×K	999.80	Joback Method
cpg	994.86	J/mol×K	1040.40	Joback Method
cpg	1021.21	J/mol×K	1080.99	Joback Method

cpg	1048.92	J/mol×K	1121.58	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=C110936782&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume