Myrtenyl formate

Inchi: InChI=1S/C11H16O2/c1-11(2)9-4-3-8(6-13-7-12)10(11)5-9/h3,7,9-10H,4-6H2,1-2H3
InchiKey: QHPJGDWWLWJMPM-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CC1(C)C2CC=C(COC=O)C1C2
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-46.25	kJ/mol	Joback Method
hf	-307.52	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	48.70	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.152		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1238.00		NIST Webbook
tb	539.62	K	Joback Method
tc	748.48	K	Joback Method
tf	343.26	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.99	J/mol×K	539.62	Joback Method
cpg	386.98	J/mol×K	574.43	Joback Method
cpg	401.95	J/mol×K	609.24	Joback Method
cpg	416.03	J/mol×K	644.05	Joback Method
cpg	429.33	J/mol×K	678.86	Joback Method
cpg	441.98	J/mol×K	713.67	Joback Method
cpg	454.10	J/mol×K	748.48	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=R233211&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

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