Myrtenyl angelate

Inchi: InChI=1S/C15H22O2/c1-5-10(2)14(16)17-9-11-6-7-12-8-13(11)15(12,3)4/h5-6,12-13H,7-
InchiKey: NVDMRTRSCKSXHT-YHYXMXQVSA-N
Formula: C15H22O2
SMILES: CC=C(C)C(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 234.33
CAS: 138530-45-7

Physical Properties

Property code	Value	Unit	Source
gf	29.70	kJ/mol	Joback Method
hf	-309.65	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.488		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1611.40		NIST Webbook
rinpol	1611.40		NIST Webbook
tb	640.39	K	Joback Method
tc	852.82	K	Joback Method
tf	377.23	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.40	J/mol×K	640.39	Joback Method
cpg	569.60	J/mol×K	675.79	Joback Method
cpg	586.84	J/mol×K	711.20	Joback Method
cpg	603.27	J/mol×K	746.60	Joback Method
cpg	619.04	J/mol×K	782.01	Joback Method
cpg	634.31	J/mol×K	817.41	Joback Method
cpg	649.22	J/mol×K	852.82	Joback Method

Sources

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=C138530457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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