Birkenyl acetate

Inchi: InChI=1S/C16H26O2/c1-11-8-16(5,10-18-12(2)17)7-6-14-13(11)9-15(14,3)4/h13-14H,1,6
InchiKey: DQIYNENWJHGCCR-OFQRWUPVSA-N
Formula: C16H26O2
SMILES: C=C1CC(C)(COC(C)=O)CCC2C1CC2(C)C
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	-38.20	kJ/mol	Joback Method
hf	-417.21	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	57.95	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.958		Crippen Method
mcvol	217.720	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
ripol	2009.00		NIST Webbook
ripol	2009.00		NIST Webbook
ripol	2009.00		NIST Webbook
tb	658.36	K	Joback Method
tc	875.14	K	Joback Method
tf	420.56	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.36	J/mol×K	658.36	Joback Method
cpg	650.47	J/mol×K	694.49	Joback Method
cpg	670.67	J/mol×K	730.62	Joback Method
cpg	690.16	J/mol×K	766.75	Joback Method
cpg	709.16	J/mol×K	802.88	Joback Method
cpg	727.87	J/mol×K	839.01	Joback Method
cpg	746.50	J/mol×K	875.14	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=R340631&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume