«alpha»-Kessyl acetate

Inchi: InChI=1S/C17H28O3/c1-10-8-14(19-11(2)18)15-13(10)9-12-6-7-17(15,5)20-16(12,3)4/h1
InchiKey: SXGDMINSYARVTP-UHFFFAOYSA-N
Formula: C17H28O3
SMILES: CC(=O)OC1CC(C)C2CC3CCC(C)(OC3(C)C)C12
Mol. weight [g/mol]: 280.40
CAS: 3925-77-7

Physical Properties

Property code	Value	Unit	Source
gf	-123.65	kJ/mol	Joback Method
hf	-621.97	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	63.82	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.558		Crippen Method
mcvol	231.120	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1820.60		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1820.60		NIST Webbook
ripol	2387.00		NIST Webbook
ripol	2387.00		NIST Webbook
tb	706.43	K	Joback Method
tc	929.31	K	Joback Method
tf	454.18	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.75	J/mol×K	706.43	Joback Method
cpg	759.02	J/mol×K	743.58	Joback Method
cpg	781.42	J/mol×K	780.72	Joback Method

cpg	803.20	J/mol×K	817.87	Joback Method
cpg	824.60	J/mol×K	855.02	Joback Method
cpg	845.88	J/mol×K	892.17	Joback Method
cpg	867.29	J/mol×K	929.31	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=C3925777&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
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