(E)-2-Methyl-6-(p-tolyl)hept-2-en-1-yl acetate

Inchi: InChI=1S/C17H24O2/c1-13-8-10-17(11-9-13)15(3)7-5-6-14(2)12-19-16(4)18/h6,8-11,15H
InchiKey: MGCGLWILILAXQZ-MKMNVTDBSA-N
Formula: C17H24O2
SMILES: CC(=O)OCC(C)=CCCC(C)c1ccc(C)cc1
Mol. weight [g/mol]: 260.37
CAS: 93125-00-9

Physical Properties

Property code	Value	Unit	Source
gf	30.35	kJ/mol	Joback Method
hf	-311.80	kJ/mol	Joback Method
hfus	31.59	kJ/mol	Joback Method
hvap	65.18	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.388		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1838.10		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1838.10		NIST Webbook
tb	699.91	K	Joback Method
tc	906.88	K	Joback Method
tf	358.41	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.07	J/mol×K	699.91	Joback Method
cpg	649.48	J/mol×K	734.41	Joback Method
cpg	665.84	J/mol×K	768.90	Joback Method
cpg	681.22	J/mol×K	803.40	Joback Method
cpg	695.65	J/mol×K	837.89	Joback Method

cpg	709.16	J/mol×K	872.39	Joback Method
cpg	721.82	J/mol×K	906.88	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=C93125009&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume