«alpha»-Santalol acetate

Inchi: InChI=1S/C17H26O2/c1-11(10-19-12(2)18)6-5-7-16(3)13-8-14-15(9-13)17(14,16)4/h6,13
InchiKey: IXRPKRWXUJOOBZ-WDZFZDKYSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC(C)=CCCC1(C)C2CC3C(C2)C31C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
hfus	29.62	kJ/mol	Joback Method
logp	3.958		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
rinpol	1756.00		NIST Webbook
rinpol	1773.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.79	J/mol×K	671.51	Joback Method
cpg	677.42	J/mol×K	705.66	Joback Method
cpg	695.36	J/mol×K	739.82	Joback Method
cpg	712.87	J/mol×K	773.97	Joback Method
cpg	730.22	J/mol×K	808.13	Joback Method
cpg	747.66	J/mol×K	842.28	Joback Method
cpg	765.44	J/mol×K	876.44	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R329387&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices