«beta»-Santanol acetate

Other names: «beta»-Santalol acetate
Inchi: InChI=1S/C17H26O2/c1-12(11-19-14(3)18)6-5-9-17(4)13(2)15-7-8-16(17)10-15/h6,15-16
InchiKey: RCFGRZLLBGMERD-WUXMJOGZSA-N
Formula: C17H26O2
SMILES: C=C1C2CCC(C2)C1(C)CCC=C(C)COC(C)=O
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
hfus	29.25	kJ/mol	Joback Method
logp	4.268		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
rinpol	1796.90		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.97	J/mol×K	681.17	Joback Method
cpg	678.12	J/mol×K	715.38	Joback Method
cpg	696.38	J/mol×K	749.59	Joback Method
cpg	713.90	J/mol×K	783.80	Joback Method
cpg	730.81	J/mol×K	818.00	Joback Method
cpg	747.25	J/mol×K	852.21	Joback Method
cpg	763.38	J/mol×K	886.42	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U132294&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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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