(Z)-«alpha»-trans-«beta»-Bergamotol acetate

Other names: cis-«alpha»-Bergamotol acetate
(Z)- «alpha»-Bergamotol acetate
Inchi: InChI=1S/C17H26O2/c1-12(11-19-14(3)18)6-5-9-17(4)15-8-7-13(2)16(17)10-15/h6-7,15-
InchiKey: BDYQEBZJCFGMCH-JBWSJSMZSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC(C)=CCCC1(C)C2CC=C(C)C1C2
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
hfus	31.24	kJ/mol	Joback Method
logp	4.268		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1790.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2296.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.76	J/mol×K	686.15	Joback Method
cpg	678.74	J/mol×K	720.52	Joback Method
cpg	696.87	J/mol×K	754.90	Joback Method
cpg	714.28	J/mol×K	789.27	Joback Method
cpg	731.12	J/mol×K	823.64	Joback Method
cpg	747.53	J/mol×K	858.02	Joback Method
cpg	763.66	J/mol×K	892.39	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R417117&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices