«alpha»-E-Bergamotyl 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	1779.00		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=R435799&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