Traseolide

Other names: 1-[2,3-dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)-1H-inden-5-yl]ethan-1-one
Traseolide
Inchi: InChI=1S/C18H26O/c1-10(2)17-12(4)18(6,7)16-8-11(3)14(13(5)19)9-15(16)17/h8-10,12,
InchiKey: IMRYETFJNLKUHK-UHFFFAOYSA-N
Formula: C18H26O
SMILES: CC(=O)c1cc2c(cc1C)C(C)(C)C(C)C2C(C)C
Mol. weight [g/mol]: 258.41

Physical Properties

Property code	Value	Unit	Source
hfus	27.31	kJ/mol	Joback Method
logp	4.865		Crippen Method
mcvol	231.430	ml/mol	McGowan Method
tf	371.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.55	J/mol×K	703.93	Joback Method
cpg	686.14	J/mol×K	739.93	Joback Method
cpg	704.87	J/mol×K	775.94	Joback Method
cpg	722.86	J/mol×K	811.94	Joback Method
cpg	740.26	J/mol×K	847.94	Joback Method
cpg	757.19	J/mol×K	883.94	Joback Method
cpg	773.80	J/mol×K	919.95	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68140487&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point