Ethanone, 1-[2,3-dihydro-1,1,2,6-tetramethyl-3-(1-methylethy

Other names: Traseolide

1-[2,3-dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)-1H-inden-5-yl]ethan-1-one

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]: 258.40

CAS: 68140-48-7

Physical Properties

Property code	Value	Unit	Source
gf	92.68	kJ/mol	Joback Method
hf	-283.23	kJ/mol	Joback Method
hfus	27.31	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.865		Crippen Method
mcvol	231.430	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
tb	703.93	K	Joback Method
tc	919.95	K	Joback Method
tf	424.89	K	Joback Method
vc	0.888	m3/kmol	Joback Method

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68140487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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