7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin

Other names:	Versalide
	Ethanone, 1-(3-ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-
	Musk 36A
	Polycyclic musk
	1,1,4,4-Tetramethyl-6-ethyl-7-acetyl-1,2,3,4-tetrahydronaphthalene
	2'-Acetonaphthone, 3'-ethyl-5',6',7',8'-tetrahydro-5',5',8',8'-tetramethyl-
	3'-Ethyl-5',6',7',8'-tetrahydro-5',5',8',8'-tetramethyl-2'-acetonaphthone
	7-Acetyl-6-ethyl-1,1,4,4-tetramethyl-1,2,3,4-tetrahydronaphthalene
	6-Acetyl-1,1,4,4-tetramethyl-7-ethyltetralin
	AETT
	1-(3-Ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-ethanone
	1,2,3,4-Tetrahydronaphthalene, 6-acetyl-7-ethyl-1,1,4,4-tetramethyl-
	1,1,4,4-Tetramethyl-6-ethyl-7-acetyltetralin
	7-Acetyl-6-ethyl-1,2,3,4-tetrahydro-1,1,4,4-tetramethylnaphthalene
	NSC 15342
Inchi:	InChI=1S/C18H26O/c1-7-13-10-15-16(11-14(13)12(2)19)18(5,6)9-8-17(15,3)4/h10-11H,7
InchiKey:	KSEZPRJUTHMFGZ-UHFFFAOYSA-N
Formula:	C18H26O
SMILES:	CCc1cc2c(cc1C(C)=O)C(C)(C)CCC2(C)C
Mol. weight [g/mol]:	258.40
CAS:	88-29-9

Physical Properties

Property code	Value	Unit	Source
gf	85.24	kJ/mol	Joback Method
hf	-248.53	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.801		Crippen Method
mcvol	231.430	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
tb	713.55	K	Joback Method
tc	939.27	K	Joback Method
tf	464.51	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.33	J/mol×K	713.55	Joback Method
cpg	682.22	J/mol×K	751.17	Joback Method
cpg	701.58	J/mol×K	788.79	Joback Method
cpg	720.66	J/mol×K	826.41	Joback Method
cpg	739.71	J/mol×K	864.03	Joback Method
cpg	758.97	J/mol×K	901.65	Joback Method
cpg	778.70	J/mol×K	939.27	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88299&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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