5-Octen-2-one, 6-methyl-8-(2,6,6-trimethyl-1-cyclohexen-1-yl)-

Inchi: InChI=1S/C18H30O/c1-14(8-6-10-16(3)19)11-12-17-15(2)9-7-13-18(17,4)5/h8H,6-7,9-13

InchiKey: JJTXQCMHUFFVOF-RIYZIHGNSA-N

Formula: C18H30O

SMILES: CC(=O)CCC=C(C)CCC1=C(C)CCCC1(C)C

Mol. weight [g/mol]: 262.43

CAS: 55638-41-0

Physical Properties

Property code	Value	Unit	Source
gf	73.09	kJ/mol	Joback Method
hf	-315.60	kJ/mol	Joback Method
hfus	28.85	kJ/mol	Joback Method
hvap	63.34	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.609		Crippen Method
mcvol	246.590	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
tb	698.06	K	Joback Method
tc	903.89	K	Joback Method
tf	380.59	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.35	J/mol×K	698.06	Joback Method
cpg	724.57	J/mol×K	732.36	Joback Method
cpg	743.90	J/mol×K	766.67	Joback Method
cpg	762.45	J/mol×K	800.97	Joback Method
cpg	780.35	J/mol×K	835.28	Joback Method
cpg	797.73	J/mol×K	869.58	Joback Method
cpg	814.71	J/mol×K	903.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55638410&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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