

8-Ketoylangenal

Inchi:	InChI=1S/C15H20O2/c1-8(2)12-11(17)6-15(3)10-5-4-9(7-16)14(15)13(10)12/h4,7-8,10,1
InchiKey:	USHAYNWHSSDBMV-UHFFFAOYSA-N
Formula:	C15H20O2
SMILES:	CC(C)C1C(=O)CC2(C)C3CC=C(C=O)C2C13
Mol. weight [g/mol]:	232.32
CAS:	136458-94-1

Physical Properties

Property code	Value	Unit	Source
gf	20.44	kJ/mol	Joback Method
hf	-348.38	kJ/mol	Joback Method
hfus	21.86	kJ/mol	Joback Method
hvap	58.66	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.629		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1825.80		NIST Webbook
rinpol	1825.80		NIST Webbook
tb	678.17	K	Joback Method
tc	906.45	K	Joback Method
tf	433.03	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.73	J/mol×K	678.17	Joback Method
cpg	586.89	J/mol×K	716.22	Joback Method
cpg	605.06	J/mol×K	754.26	Joback Method
cpg	622.44	J/mol×K	792.31	Joback Method
cpg	639.18	J/mol×K	830.36	Joback Method
cpg	655.48	J/mol×K	868.40	Joback Method
cpg	671.52	J/mol×K	906.45	Joback Method

Sources

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=C136458941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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