Dihydrojasmone

Other names:	2-Cyclopenten-1-one, 3-methyl-2-pentyl-
	Jasmone, dihydro-
	3-Methyl-2-(n-pentanyl)-2-cyclopenten-1-one
	2-Pentyl-3-methyl-2-cyclopenten-1-one
	2-n-Pentyl-3-methyl-2-cyclopenten-1-one
	3-methyl-2-pentylcyclopent-2-enone
Inchi:	InChI=1S/C11H18O/c1-3-4-5-6-10-9(2)7-8-11(10)12/h3-8H2,1-2H3
InchiKey:	YCIXWYOBMVNGTB-UHFFFAOYSA-N
Formula:	C11H18O
SMILES:	CCCCCC1=C(C)CCC1=O
Mol. weight [g/mol]:	166.26
CAS:	1128-08-1

Physical Properties

Property code	Value	Unit	Source
gf	-25.89	kJ/mol	Joback Method
hf	-292.41	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	46.51	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.246		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1362.40		NIST Webbook
ripol	1842.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	547.97	K	Joback Method
tc	755.00	K	Joback Method
tf	322.89	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.24	J/mol×K	547.97	Joback Method
cpg	383.69	J/mol×K	582.48	Joback Method
cpg	399.40	J/mol×K	616.98	Joback Method
cpg	414.36	J/mol×K	651.49	Joback Method
cpg	428.57	J/mol×K	685.99	Joback Method
cpg	442.06	J/mol×K	720.50	Joback Method
cpg	454.82	J/mol×K	755.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.70	K	2.90	NIST Webbook
tbrp	389.20	K	1.60	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1128081&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume