3-METHYL-2-PENTYLCYCLOPENT-2-ENONE

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

Physical Properties

Property code	Value	Unit	Source
hfus	17.06	kJ/mol	Joback Method
logp	3.246		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
rinpol	1362.40		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1362.40		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1842.00		NIST Webbook
ripol	1892.00		NIST Webbook

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: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1128081&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tbrp: Boiling point at reduced pressure

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