trans-Jasmone

Other names:	(E)-Jasmone
	3-methyl-2-(trans-2-pentenyl)-2-cyclopenten-1-one
	(E)-3-methyl-2-(pent-2-enyl)cyclopent-2-en-1-one
Inchi:	InChI=1S/C11H16O/c1-3-4-5-6-10-9(2)7-8-11(10)12/h4-5H,3,6-8H2,1-2H3/b5-4+
InchiKey:	XMLSXPIVAXONDL-SNAWJCMRSA-N
Formula:	C11H16O
SMILES:	CCC=CCC1=C(C)CCC1=O
Mol. weight [g/mol]:	164.24
CAS:	6261-18-3

Physical Properties

Property code	Value	Unit	Source
gf	54.33	kJ/mol	Joback Method
hf	-175.19	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	46.47	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.022		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1385.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	1948.00		NIST Webbook
tb	552.13	K	Joback Method
tc	768.56	K	Joback Method
tf	317.81	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.55	J/mol×K	552.13	Joback Method
cpg	364.59	J/mol×K	588.20	Joback Method
cpg	379.80	J/mol×K	624.27	Joback Method
cpg	394.21	J/mol×K	660.34	Joback Method
cpg	407.84	J/mol×K	696.41	Joback Method
cpg	420.71	J/mol×K	732.49	Joback Method
cpg	432.85	J/mol×K	768.56	Joback Method

Sources

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=C6261183&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume