trans-Dihydrojasmone

Inchi: InChI=1S/C11H18O/c1-3-4-5-6-10-9(2)7-8-11(10)12/h4-5,9-10H,3,6-8H2,1-2H3/b5-4-/t9-

InchiKey: QQLJHNUFLMPPGC-YVDHIRPGSA-N

Formula: C11H18O

SMILES: CCC=CCC1C(=O)CCC1C

Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	28.21	kJ/mol	Joback Method
hf	-250.71	kJ/mol	Joback Method
hfus	18.96	kJ/mol	Joback Method
hvap	44.23	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.958		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	533.67	K	Joback Method
tc	745.61	K	Joback Method
tf	283.53	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.74	J/mol×K	533.67	Joback Method
cpg	387.43	J/mol×K	568.99	Joback Method
cpg	405.18	J/mol×K	604.32	Joback Method
cpg	422.01	J/mol×K	639.64	Joback Method
cpg	437.95	J/mol×K	674.97	Joback Method
cpg	453.00	J/mol×K	710.29	Joback Method

cpg	467.19	J/mol×K	745.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410334&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
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