(E,E)-Farnesyl acetone

Inchi: InChI=1S/C18H28O/c1-15(2)9-6-10-16(3)11-7-12-17(4)13-8-14-18(5)19/h8-9,11,13-14H,
InchiKey: HGFAGNRYCRACAH-WWESEOGYSA-N
Formula: C18H28O
SMILES: CC(=O)C=CC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 260.41

Physical Properties

Property code	Value	Unit	Source
gf	266.99	kJ/mol	Joback Method
hf	-87.92	kJ/mol	Joback Method
hfus	40.85	kJ/mol	Joback Method
hvap	62.48	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.551		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	1919.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1915.00		NIST Webbook
ripol	2382.00		NIST Webbook
ripol	2382.00		NIST Webbook
ripol	2377.00		NIST Webbook
tb	681.39	K	Joback Method
tc	876.63	K	Joback Method
tf	280.35	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.46	J/mol×K	681.39	Joback Method
cpg	688.34	J/mol×K	713.93	Joback Method
cpg	705.27	J/mol×K	746.47	Joback Method
cpg	721.34	J/mol×K	779.01	Joback Method
cpg	736.62	J/mol×K	811.55	Joback Method
cpg	751.20	J/mol×K	844.09	Joback Method
cpg	765.16	J/mol×K	876.63	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=R287000&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