(E,Z)-Farnesal

Inchi: InChI=1S/C15H24O/c1-13(2)7-5-8-14(3)9-6-10-15(4)11-12-16/h7,9,11-12H,5-6,8,10H2,1
InchiKey: YHRUHBBTQZKMEX-GNESMGCMSA-N
Formula: C15H24O
SMILES: CC(C)=CCCC(C)=CCCC(C)=CC=O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	190.91	kJ/mol	Joback Method
hf	-116.22	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	55.82	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.605		Crippen Method
mcvol	210.880	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
ripol	2225.00		NIST Webbook
tb	603.38	K	Joback Method
tc	794.15	K	Joback Method
tf	243.69	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.64	J/mol×K	603.38	Joback Method
cpg	547.51	J/mol×K	635.18	Joback Method
cpg	563.47	J/mol×K	666.97	Joback Method
cpg	578.59	J/mol×K	698.77	Joback Method
cpg	592.93	J/mol×K	730.56	Joback Method
cpg	606.55	J/mol×K	762.36	Joback Method
cpg	619.50	J/mol×K	794.15	Joback Method

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=R327861&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume