(E,E)-«alpha»-Farnesene

Inchi: InChI=1S/C15H24/c1-6-14(4)10-8-12-15(5)11-7-9-13(2)3/h6,9-10,12H,1,7-8,11H2,2-5H3
InchiKey: CXENHBSYCFFKJS-VDQVFBMKSA-N
Formula: C15H24
SMILES: C=CC(C)=CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hf	-7.48	kJ/mol	Cheméo Relay (1.0)
hfus	30.00	kJ/mol	Joback Method
hvap	66.81	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.65		Cheméo Relay (1.0)
logp	5.202		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinpol	1507.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1505.00		NIST Webbook

rinpol	1509.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1506.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1757.00		NIST Webbook
ripol	1740.00		NIST Webbook
tb	526.53	K	Cheméo Relay (1.0)
tf	224.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.77	J/mol×K	551.40	Joback Method
cpg	501.93	J/mol×K	583.16	Joback Method
cpg	519.09	J/mol×K	614.93	Joback Method
cpg	535.33	J/mol×K	646.69	Joback Method
cpg	550.70	J/mol×K	678.45	Joback Method
cpg	565.26	J/mol×K	710.22	Joback Method
cpg	579.10	J/mol×K	741.98	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=R601822&Units=SI

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point