(E)-«beta»-Farnesene

Inchi: InChI=1S/C15H24/c1-6-14(4)10-8-12-15(5)11-7-9-13(2)3/h6,9,12H,1,4,7-8,10-11H2,2-3,5
InchiKey: JSNRRGGBADWTMC-NTCAYCPXSA-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	-11.45	kJ/mol	Cheméo Relay (1.0)
hfus	28.52	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.40		Cheméo Relay (1.0)
logp	5.202		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinpol	1460.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1452.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1673.00		NIST Webbook

ripol	1660.00		NIST Webbook
tb	518.76	K	Cheméo Relay (1.0)
tf	212.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.95	J/mol×K	543.92	Joback Method
cpg	499.95	J/mol×K	574.97	Joback Method
cpg	517.00	J/mol×K	606.02	Joback Method
cpg	533.16	J/mol×K	637.07	Joback Method
cpg	548.48	J/mol×K	668.12	Joback Method
cpg	563.01	J/mol×K	699.17	Joback Method
cpg	576.82	J/mol×K	730.22	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R601164&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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