«beta»-(Z)-Farnesene

Inchi: InChI=1S/C16H26/c1-6-15(4)12-9-13-16(5)11-8-7-10-14(2)3/h6,10,13H,1,4,7-9,11-12H2,
InchiKey: KMRFPAWPLWBTJN-SSZFMOIBSA-N
Formula: C16H26
SMILES: C=CC(=C)CCC=C(C)CCCC=C(C)C
Mol. weight [g/mol]: 218.38

Physical Properties

Property code	Value	Unit	Source
hfus	31.11	kJ/mol	Joback Method
hvap	70.30	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.76		Cheméo Relay (1.0)
logp	5.592		Crippen Method
mcvol	219.100	ml/mol	McGowan Method
rinpol	1438.00		NIST Webbook
tb	533.92	K	Cheméo Relay (1.0)
tf	223.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.94	J/mol×K	566.80	Joback Method
cpg	551.39	J/mol×K	597.51	Joback Method
cpg	568.90	J/mol×K	628.22	Joback Method
cpg	585.50	J/mol×K	658.94	Joback Method
cpg	601.27	J/mol×K	689.65	Joback Method
cpg	616.25	J/mol×K	720.36	Joback Method
cpg	630.50	J/mol×K	751.07	Joback Method

Sources

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=R616854&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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point