«beta»-(E)-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	1454.00		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

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=R616829&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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point