trans, trans-«beta»-farnesene

Other names: (E,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	-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	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1727.00		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

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308360&Units=SI

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

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