trans-«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	1441.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1444.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1667.00		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: 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=R600527&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
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