«beta»-(E)-Guaiene

Inchi: InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h11-12H,5-9H2,1-4H3/t1
InchiKey: GIBQERSGRNPMEH-NWDGAFQWSA-N
Formula: C15H24
SMILES: CC(C)=C1CCC(C)C2=C(C1)C(C)CC2
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	21.93	kJ/mol	Joback Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1498.00		NIST Webbook
tb	540.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.31	J/mol×K	588.80	Joback Method
cpg	525.51	J/mol×K	625.37	Joback Method
cpg	546.40	J/mol×K	661.93	Joback Method
cpg	566.04	J/mol×K	698.50	Joback Method
cpg	584.49	J/mol×K	735.06	Joback Method
cpg	601.81	J/mol×K	771.63	Joback Method
cpg	618.07	J/mol×K	808.19	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=R616834&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature