«alpha»2-bisabolene

Other names: Prenyllimonene
Inchi: InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6-8,15H,5,9-11H2,1-4H3/b
InchiKey: YHBUQBJHSRGZNF-AUWJEWJLSA-N
Formula: C15H24
SMILES: CC(C)=CCC=C(C)C1CC=C(C)CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	25.06	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Cheméo Relay (1.0)
ie	8.00	eV	Cheméo Relay (1.0)
log10ws	-5.83		Cheméo Relay (1.0)
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
rinpol	1436.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1508.00		NIST Webbook
ripol	1736.00		NIST Webbook
tb	543.96	K	Cheméo Relay (1.0)
tf	244.28	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.01	J/mol×K	574.37	Joback Method
cpg	516.16	J/mol×K	609.64	Joback Method
cpg	536.07	J/mol×K	644.90	Joback Method
cpg	554.80	J/mol×K	680.17	Joback Method
cpg	572.42	J/mol×K	715.43	Joback Method
cpg	589.00	J/mol×K	750.70	Joback Method
cpg	604.60	J/mol×K	785.97	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R209426&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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