(Z)-«gamma»-Bisabolene

Inchi: InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8H,5,7,9-11H2,1-4H3/b1
InchiKey: XBGUIVFBMBVUEG-CCEZHUSRSA-N
Formula: C15H24
SMILES: CC(C)=CCCC(C)=C1CC=C(C)CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	24.11	kJ/mol	Joback Method
logp	5.179		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
rinpol	1514.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1512.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.12	J/mol×K	581.52	Joback Method
cpg	514.12	J/mol×K	616.38	Joback Method
cpg	532.97	J/mol×K	651.24	Joback Method
cpg	550.75	J/mol×K	686.10	Joback Method
cpg	567.52	J/mol×K	720.96	Joback Method
cpg	583.32	J/mol×K	755.82	Joback Method
cpg	598.22	J/mol×K	790.68	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=R610752&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