

(6R,7R)-Bisabolone

Inchi:	InChI=1S/C15H24O/c1-11(2)6-5-7-13(4)14-9-8-12(3)10-15(14)16/h6,10,13-14H,5,7-9H2,
InchiKey:	KNOUERLLBMJGLF-ZIAGYGMSSA-N
Formula:	C15H24O
SMILES:	CC(C)=CCCC(C)C1CCC(C)=CC1=O
Mol. weight [g/mol]:	220.35
CAS:	72441-71-5

Physical Properties

Property code	Value	Unit	Source
gf	66.84	kJ/mol	Joback Method
hf	-287.85	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.294		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1755.00		NIST Webbook
ripol	2320.00		NIST Webbook
tb	637.71	K	Joback Method
tc	853.69	K	Joback Method
tf	313.65	K	Joback Method
vc	0.776	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.22	J/mol×K	637.71	Joback Method

cpg	575.88	J/mol×K	673.71	Joback Method
cpg	595.37	J/mol×K	709.70	Joback Method
cpg	613.70	J/mol×K	745.70	Joback Method
cpg	630.91	J/mol×K	781.70	Joback Method
cpg	647.03	J/mol×K	817.69	Joback Method
cpg	662.08	J/mol×K	853.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72441715&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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