(6S,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-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC(C)=CCCC(C)C1CCC(C)=CC1=O
Mol. weight [g/mol]: 220.35
CAS: 72441-70-4

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	1754.50		NIST Webbook
rinpol	1754.50		NIST Webbook
rinpol	1754.50		NIST Webbook
tb	637.71	K	Joback Method
tc	853.69	K	Joback Method
tf	313.65	K	Joback Method
vc	0.776	m3/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

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=C72441704&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume