«beta»-Bisabolenal

Inchi: InChI=1S/C15H22O/c1-12(2)5-4-6-13(3)15-9-7-14(11-16)8-10-15/h5,7,11,15H,3-4,6,8-10
InchiKey: JZLKKMAUZMMUMS-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(CCC=C(C)C)C1CC=C(C=O)CC1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	171.64	kJ/mol	Joback Method
hf	-114.81	kJ/mol	Joback Method
hfus	25.86	kJ/mol	Joback Method
hvap	56.53	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1738.00		NIST Webbook
ripol	2380.00		NIST Webbook
tb	615.55	K	Joback Method
tc	825.26	K	Joback Method
tf	286.71	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.08	J/mol×K	615.55	Joback Method
cpg	538.97	J/mol×K	650.50	Joback Method
cpg	556.74	J/mol×K	685.45	Joback Method
cpg	573.43	J/mol×K	720.40	Joback Method
cpg	589.10	J/mol×K	755.35	Joback Method
cpg	603.81	J/mol×K	790.30	Joback Method

cpg	617.62	J/mol×K	825.26	Joback Method

Sources

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=R234398&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume