Bisabol-1-one

Inchi: InChI=1S/C15H28O/c1-11(2)6-5-7-13(4)14-9-8-12(3)10-15(14)16/h11-14H,5-10H2,1-4H3
InchiKey: KCRFTEABMBVXDT-UHFFFAOYSA-N
Formula: C15H28O
SMILES: CC(C)CCCC(C)C1CCC(C)CC1=O
Mol. weight [g/mol]: 224.38

Physical Properties

Property code	Value	Unit	Source
gf	-35.31	kJ/mol	Joback Method
hf	-467.21	kJ/mol	Joback Method
hfus	19.98	kJ/mol	Joback Method
hvap	52.58	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.454		Crippen Method
mcvol	212.920	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1754.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1713.00		NIST Webbook
tb	624.42	K	Joback Method
tc	829.91	K	Joback Method
tf	300.17	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.08	J/mol×K	624.42	Joback Method
cpg	621.90	J/mol×K	658.67	Joback Method
cpg	643.52	J/mol×K	692.92	Joback Method
cpg	663.95	J/mol×K	727.17	Joback Method
cpg	683.20	J/mol×K	761.42	Joback Method
cpg	701.27	J/mol×K	795.66	Joback Method
cpg	718.18	J/mol×K	829.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R424021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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