3-Hydroxybisabola-1(6)-dien-2-one B

Inchi: InChI=1S/C15H26O2/c1-11(2)6-5-7-12(3)13-8-9-15(4,17)14(16)10-13/h10-12,17H,5-9H2
InchiKey: OXQXZFFVWPEAHX-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: CC(C)CCCC(C)C1=CC(=O)C(C)(O)CC1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-149.58	kJ/mol	Joback Method
hf	-537.55	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	69.37	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.489		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
ripol	2487.00		NIST Webbook
ripol	2487.00		NIST Webbook
tb	725.65	K	Joback Method
tc	928.31	K	Joback Method
tf	402.41	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.27	J/mol×K	725.65	Joback Method
cpg	660.91	J/mol×K	759.43	Joback Method
cpg	677.82	J/mol×K	793.20	Joback Method
cpg	694.08	J/mol×K	826.98	Joback Method
cpg	709.76	J/mol×K	860.76	Joback Method
cpg	724.96	J/mol×K	894.54	Joback Method

cpg	739.74	J/mol×K	928.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R395681&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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