Modhephen-8«beta»-ol

Inchi: InChI=1S/C15H24O/c1-11-10-12(2,3)14-6-5-7-15(11,14)13(4,16)8-9-14/h10,16H,5-9H2,1
InchiKey: WAFFJCDTFBFQCN-KKUMJFAQSA-N
Formula: C15H24O
SMILES: CC1=CC(C)(C)C23CCCC12C(C)(O)CC3
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	87.31	kJ/mol	Joback Method
hf	-212.15	kJ/mol	Joback Method
hfus	5.61	kJ/mol	Joback Method
hvap	61.79	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.674		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1514.00		NIST Webbook
tb	663.97	K	Joback Method
tc	887.90	K	Joback Method
tf	471.05	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.30	J/mol×K	663.97	Joback Method
cpg	583.16	J/mol×K	701.29	Joback Method
cpg	600.73	J/mol×K	738.61	Joback Method
cpg	618.48	J/mol×K	775.94	Joback Method
cpg	636.91	J/mol×K	813.26	Joback Method
cpg	656.50	J/mol×K	850.58	Joback Method
cpg	677.73	J/mol×K	887.90	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=R641444&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