Davanone C

Inchi: InChI=1S/C15H24O2/c1-6-15(5)10-9-14(17-15)12(4)13(16)8-7-11(2)3/h6-7,12,14H,1,8-1
InchiKey: FJKKZNIYYVEYOL-JENMUQSASA-N
Formula: C15H24O2
SMILES: C=CC1(C)CCC(C(C)C(=O)CC=C(C)C)O1
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	40.80	kJ/mol	Joback Method
hf	-314.55	kJ/mol	Joback Method
hfus	26.98	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.672		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1526.00		NIST Webbook
tb	634.55	K	Joback Method
tc	845.68	K	Joback Method
tf	330.07	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.19	J/mol×K	634.55	Joback Method
cpg	592.37	J/mol×K	669.74	Joback Method
cpg	610.50	J/mol×K	704.93	Joback Method
cpg	627.73	J/mol×K	740.11	Joback Method
cpg	644.19	J/mol×K	775.30	Joback Method
cpg	660.02	J/mol×K	810.49	Joback Method
cpg	675.35	J/mol×K	845.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R226718&Units=SI

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