zierone(elleryone)

Inchi: InChI=1S/C15H22O/c1-9(2)14-13(16)8-6-10(3)12-7-5-11(4)15(12)14/h10,12H,5-8H2,1-4
InchiKey: OONKKRRSPIDEBA-JQWIXIFHSA-N
Formula: C15H22O
SMILES: CC(C)=C1C(=O)CCC(C)C2CCC(C)=C12
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	73.54	kJ/mol	Joback Method
hf	-268.59	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1754.00		NIST Webbook
tb	656.62	K	Joback Method
tc	888.37	K	Joback Method
tf	371.03	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.57	J/mol×K	656.62	Joback Method
cpg	563.73	J/mol×K	695.24	Joback Method
cpg	583.58	J/mol×K	733.87	Joback Method
cpg	602.15	J/mol×K	772.49	Joback Method
cpg	619.47	J/mol×K	811.12	Joback Method
cpg	635.58	J/mol×K	849.74	Joback Method
cpg	650.50	J/mol×K	888.37	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=R519976&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