1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3

Other names: Vertofix coeur
Inchi: InChI=1S/C17H26O/c1-10-6-7-15-16(4,5)14-9-17(10,15)8-13(11(14)2)12(3)18/h10,14-15
InchiKey: YBUIAJZFOGJGLJ-UHFFFAOYSA-N
Formula: C17H26O
SMILES: CC(=O)C1=C(C)C2CC3(C1)C(C)CCC3C2(C)C
Mol. weight [g/mol]: 246.39
CAS: 68039-35-0

Physical Properties

Property code	Value	Unit	Source
gf	105.69	kJ/mol	Joback Method
hf	-276.07	kJ/mol	Joback Method
hfus	21.58	kJ/mol	Joback Method
hvap	58.96	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.374		Crippen Method
mcvol	215.080	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	1779.80		NIST Webbook
rinpol	1779.80		NIST Webbook
tb	671.25	K	Joback Method
tc	896.20	K	Joback Method
tf	443.18	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.03	J/mol×K	671.25	Joback Method
cpg	660.42	J/mol×K	708.74	Joback Method
cpg	680.93	J/mol×K	746.23	Joback Method
cpg	700.85	J/mol×K	783.72	Joback Method
cpg	720.46	J/mol×K	821.21	Joback Method
cpg	740.05	J/mol×K	858.71	Joback Method

cpg	759.92	J/mol×K	896.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68039350&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume