3,4,10,11-Tetradehydrocadinan-8-one

Inchi: InChI=1S/C15H22O/c1-9(2)15-13-7-10(3)5-6-12(13)11(4)8-14(15)16/h7,9,12-13,15H,4-6
InchiKey: UDWPGSSJAAPTCK-SSDMNJCBSA-N
Formula: C15H22O
SMILES: C=C1CC(=O)C(C(C)C)C2C=C(C)CCC12
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	89.19	kJ/mol	Joback Method
hf	-264.74	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.760		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1692.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2224.00		NIST Webbook
ripol	2224.00		NIST Webbook
tb	639.17	K	Joback Method
tc	866.07	K	Joback Method
tf	356.55	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.23	J/mol×K	639.17	Joback Method
cpg	565.16	J/mol×K	676.99	Joback Method
cpg	585.76	J/mol×K	714.80	Joback Method
cpg	605.04	J/mol×K	752.62	Joback Method

cpg	623.01	J/mol×K	790.44	Joback Method
cpg	639.71	J/mol×K	828.25	Joback Method
cpg	655.13	J/mol×K	866.07	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=R320964&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume