4a«beta»-Methyl-3,4,4a,5,6,7,8a«alpha»-hexahydr

Inchi: InChI=1S/C11H16O2/c1-11-5-2-3-10(13)9(11)7-8(12)4-6-11/h9H,2-7H2,1H3/t9-,11+/m1/s
InchiKey: PQTSRSJNADEALT-KOLCDFICSA-N
Formula: C11H16O2
SMILES: CC12CCCC(=O)C1CC(=O)CC2
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-135.83	kJ/mol	Joback Method
hf	-409.57	kJ/mol	Joback Method
hfus	4.84	kJ/mol	Joback Method
hvap	47.94	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.115		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
ripol	1927.00		NIST Webbook
tb	617.52	K	Joback Method
tc	876.60	K	Joback Method
tf	395.87	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.97	J/mol×K	617.52	Joback Method
cpg	428.79	J/mol×K	660.70	Joback Method
cpg	448.35	J/mol×K	703.88	Joback Method
cpg	466.79	J/mol×K	747.06	Joback Method
cpg	484.23	J/mol×K	790.24	Joback Method
cpg	500.80	J/mol×K	833.42	Joback Method
cpg	516.64	J/mol×K	876.60	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=R640936&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume