2-((2R,4aR,8aS)-4a-Methyl-8-methylenedecahydro

Inchi: InChI=1S/C15H22O/c1-11-5-4-7-15(3)8-6-13(9-14(11)15)12(2)10-16/h10,13-14H,1-2,4-9
InchiKey: QTCANKDTWWSCMR-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(C=O)C1CCC2(C)CCCC(=C)C2C1
Mol. weight [g/mol]: 218.33
CAS: 3650-40-6

Physical Properties

Property code	Value	Unit	Source
gf	168.17	kJ/mol	Joback Method
hf	-122.77	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	54.33	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	1691.40		NIST Webbook
rinpol	1691.40		NIST Webbook
tb	613.11	K	Joback Method
tc	838.98	K	Joback Method
tf	340.23	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.60	J/mol×K	613.11	Joback Method
cpg	547.91	J/mol×K	650.75	Joback Method
cpg	567.89	J/mol×K	688.40	Joback Method
cpg	586.72	J/mol×K	726.04	Joback Method
cpg	604.55	J/mol×K	763.69	Joback Method
cpg	621.54	J/mol×K	801.33	Joback Method
cpg	637.86	J/mol×K	838.98	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=C3650406&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