(3R,3aR,4aS,5R,9aS)-3,5,8-Trimethyl-3a,4,4a,5,6,7,

Inchi: InChI=1S/C15H22O2/c1-8-4-5-11-9(2)6-14-13(7-12(8)11)10(3)15(16)17-14/h8,10,12-14H
InchiKey: LGGWYHIMEGQREQ-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CC1=C2CCC(C)C2CC2C(C1)OC(=O)C2C
Mol. weight [g/mol]: 234.33
CAS: 66873-38-9

Physical Properties

Property code	Value	Unit	Source
gf	-4.16	kJ/mol	Joback Method
hf	-434.71	kJ/mol	Joback Method
hfus	30.69	kJ/mol	Joback Method
hvap	59.17	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.320		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1899.00		NIST Webbook
rinpol	1918.30		NIST Webbook
rinpol	1899.00		NIST Webbook
rinpol	1918.30		NIST Webbook
tb	674.45	K	Joback Method
tc	908.22	K	Joback Method
tf	410.66	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.32	J/mol×K	674.45	Joback Method
cpg	611.80	J/mol×K	713.41	Joback Method
cpg	632.78	J/mol×K	752.37	Joback Method
cpg	652.31	J/mol×K	791.34	Joback Method
cpg	670.44	J/mol×K	830.30	Joback Method

cpg	687.21	J/mol×K	869.26	Joback Method
cpg	702.67	J/mol×K	908.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66873389&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

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