trans-2-Isopropylbicylclo[4.3.0]non-3-ene-8-one

Other names: Trans-2-isopropyl-bicyclo-[4,3,0]-non-3-ene-8-one
Inchi: InChI=1S/C12H18O/c1-8(2)11-5-3-4-9-6-10(13)7-12(9)11/h3,5,8-9,11-12H,4,6-7H2,1-2H
InchiKey: MNCSLWSQTFQICJ-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC(C)C1C=CCC2CC(=O)CC21
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	32.58	kJ/mol	Joback Method
hf	-269.43	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	46.49	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.814		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
tb	562.12	K	Joback Method
tc	791.49	K	Joback Method
tf	300.06	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.35	J/mol×K	562.12	Joback Method
cpg	426.54	J/mol×K	600.35	Joback Method
cpg	446.45	J/mol×K	638.58	Joback Method
cpg	465.12	J/mol×K	676.81	Joback Method
cpg	482.59	J/mol×K	715.03	Joback Method
cpg	498.88	J/mol×K	753.26	Joback Method
cpg	514.05	J/mol×K	791.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U64600&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume