Longipinocarvone

Inchi: InChI=1S/C15H22O/c1-9-11(16)8-10-13-12(9)15(10,4)7-5-6-14(13,2)3/h10,12-13H,1,5-8
InchiKey: MIJOZYYZCMBCHF-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C1C(=O)CC2C3C1C2(C)CCCC3(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	137.56	kJ/mol	Joback Method
hf	-210.51	kJ/mol	Joback Method
hfus	12.71	kJ/mol	Joback Method
hvap	50.55	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	629.48	K	Joback Method
tc	866.95	K	Joback Method
tf	426.81	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.93	J/mol×K	629.48	Joback Method
cpg	563.88	J/mol×K	669.06	Joback Method
cpg	584.68	J/mol×K	708.64	Joback Method
cpg	604.63	J/mol×K	748.22	Joback Method
cpg	624.03	J/mol×K	787.79	Joback Method
cpg	643.18	J/mol×K	827.37	Joback Method
cpg	662.38	J/mol×K	866.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U151871&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume