trans-«gamma»-jasmine lactone

Inchi: InChI=1S/C10H16O2/c1-2-3-4-6-9-7-5-8-10(11)12-9/h2-3,9H,4-8H2,1H3/b3-2+
InchiKey: NBCMACYORPIYNY-NSCUHMNNSA-N
Formula: C10H16O2
SMILES: CC=CCCC1CCCC(=O)O1
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-70.72	kJ/mol	Joback Method
hf	-347.89	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	47.00	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.438		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
ripol	2163.00		NIST Webbook
ripol	2163.00		NIST Webbook
tb	546.68	K	Joback Method
tc	768.27	K	Joback Method
tf	299.55	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.63	J/mol×K	546.68	Joback Method
cpg	370.48	J/mol×K	583.61	Joback Method
cpg	387.36	J/mol×K	620.54	Joback Method
cpg	403.30	J/mol×K	657.48	Joback Method
cpg	418.31	J/mol×K	694.41	Joback Method
cpg	432.39	J/mol×K	731.34	Joback Method
cpg	445.57	J/mol×K	768.27	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=R327396&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