

«gamma»-tridecalactone

Inchi:	InChI=1S/C13H24O2/c1-2-3-4-5-6-7-8-9-12-10-11-13(14)15-12/h12H,2-11H2,1H3
InchiKey:	JKAJPOOMLFHWAY-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	CCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]:	212.33

Physical Properties

Property code	Value	Unit	Source
gf	-113.58	kJ/mol	Joback Method
hf	-520.87	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.833		Crippen Method
mvol	190.610	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
ripol	2488.00		NIST Webbook
ripol	2488.00		NIST Webbook
tb	606.89	K	Joback Method
tc	802.87	K	Joback Method
tf	341.96	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.19	J/mol×K	606.89	Joback Method
cpg	541.19	J/mol×K	639.55	Joback Method
cpg	559.25	J/mol×K	672.22	Joback Method
cpg	576.40	J/mol×K	704.88	Joback Method
cpg	592.65	J/mol×K	737.55	Joback Method
cpg	608.00	J/mol×K	770.21	Joback Method
cpg	622.48	J/mol×K	802.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R332388&Units=SI

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

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