(Z)-6-Dodecene-7-lactone

Inchi: InChI=1S/C12H20O2/c1-2-3-5-8-11-9-6-4-7-10-12(13)14-11/h9H,2-8,10H2,1H3/b11-9-
InchiKey: KBMKBYARCSCTRK-LUAWRHEFSA-N
Formula: C12H20O2
SMILES: CCCCCC1=CCCCCC(=O)O1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-130.26	kJ/mol	Joback Method
hf	-452.06	kJ/mol	Joback Method
hfus	21.72	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.568		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
ripol	2398.00		NIST Webbook
ripol	2398.00		NIST Webbook
tb	605.63	K	Joback Method
tc	827.95	K	Joback Method
tf	337.65	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.29	J/mol×K	605.63	Joback Method
cpg	472.93	J/mol×K	642.68	Joback Method
cpg	491.47	J/mol×K	679.74	Joback Method
cpg	508.91	J/mol×K	716.79	Joback Method
cpg	525.24	J/mol×K	753.84	Joback Method
cpg	540.44	J/mol×K	790.89	Joback Method
cpg	554.51	J/mol×K	827.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341090&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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