4-Methyl-4-decanolide

Inchi: InChI=1S/C11H20O2/c1-3-4-5-6-8-11(2)9-7-10(12)13-11/h3-9H2,1-2H3
InchiKey: ALWUKGXLBSQSMA-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: CCCCCCC1(C)CCC(=O)O1
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-135.91	kJ/mol	Joback Method
hf	-464.35	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	47.94	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.053		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2060.00		NIST Webbook
tb	561.37	K	Joback Method
tc	770.73	K	Joback Method
tf	343.32	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.15	J/mol×K	561.37	Joback Method
cpg	435.86	J/mol×K	596.26	Joback Method
cpg	452.67	J/mol×K	631.16	Joback Method
cpg	468.64	J/mol×K	666.05	Joback Method
cpg	483.86	J/mol×K	700.94	Joback Method
cpg	498.42	J/mol×K	735.84	Joback Method

cpg	512.41	J/mol×K	770.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R434716&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume