5-Methyl-5-nonanolide

Inchi: InChI=1S/C10H18O2/c1-3-4-7-10(2)8-5-6-9(11)12-10/h3-8H2,1-2H3
InchiKey: MPQRKJBKDZBMLT-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCCCC1(C)CCCC(=O)O1
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-156.43	kJ/mol	Joback Method
hf	-449.87	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	45.89	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.662		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1397.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	542.76	K	Joback Method
tc	763.32	K	Joback Method
tf	328.53	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.32	J/mol×K	542.76	Joback Method
cpg	388.37	J/mol×K	579.52	Joback Method
cpg	405.43	J/mol×K	616.28	Joback Method
cpg	421.60	J/mol×K	653.04	Joback Method
cpg	436.95	J/mol×K	689.80	Joback Method
cpg	451.58	J/mol×K	726.56	Joback Method
cpg	465.57	J/mol×K	763.32	Joback Method

Sources

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=R434776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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