5-Methyl-5-heptanolide

Inchi: InChI=1S/C8H14O2/c1-3-8(2)6-4-5-7(9)10-8/h3-6H2,1-2H3
InchiKey: JIHAIGGLAMOQBF-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CCC1(C)CCCC(=O)O1
Mol. weight [g/mol]: 142.20

Physical Properties

Property code	Value	Unit	Source
gf	-173.27	kJ/mol	Joback Method
hf	-408.59	kJ/mol	Joback Method
hfus	9.50	kJ/mol	Joback Method
hvap	41.44	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.882		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1200.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1858.00		NIST Webbook
tb	497.00	K	Joback Method
tc	725.51	K	Joback Method
tf	305.99	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.67	J/mol×K	497.00	Joback Method
cpg	294.07	J/mol×K	535.08	Joback Method
cpg	309.50	J/mol×K	573.17	Joback Method
cpg	324.05	J/mol×K	611.25	Joback Method
cpg	337.81	J/mol×K	649.34	Joback Method
cpg	350.87	J/mol×K	687.42	Joback Method
cpg	363.32	J/mol×K	725.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R434761&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
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