4-Ethyl-4-heptanolide

Inchi: InChI=1S/C9H16O2/c1-3-6-9(4-2)7-5-8(10)11-9/h3-7H2,1-2H3
InchiKey: XKLQXGYXLHWLED-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CCCC1(CC)CCC(=O)O1
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-152.75	kJ/mol	Joback Method
hf	-423.07	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	43.49	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.272		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1853.00		NIST Webbook
tb	515.61	K	Joback Method
tc	731.94	K	Joback Method
tf	320.78	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.89	J/mol×K	515.61	Joback Method
cpg	339.16	J/mol×K	551.66	Joback Method
cpg	354.51	J/mol×K	587.72	Joback Method
cpg	369.04	J/mol×K	623.77	Joback Method
cpg	382.83	J/mol×K	659.83	Joback Method
cpg	395.96	J/mol×K	695.88	Joback Method

cpg	408.53	J/mol×K	731.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R434687&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