

5-Methyl-5-octanolide

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

Physical Properties

Property code	Value	Unit	Source
gf	-164.85	kJ/mol	Joback Method
hf	-429.23	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	43.66	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.272		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1295.00		NIST Webbook
ripol	1950.00		NIST Webbook
tb	519.88	K	Joback Method
tc	744.39	K	Joback Method
tf	317.26	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.10	J/mol×K	519.88	Joback Method
cpg	340.38	J/mol×K	557.30	Joback Method
cpg	356.69	J/mol×K	594.72	Joback Method
cpg	372.10	J/mol×K	632.13	Joback Method
cpg	386.71	J/mol×K	669.55	Joback Method
cpg	400.60	J/mol×K	706.97	Joback Method
cpg	413.87	J/mol×K	744.39	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=R434781&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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