Heptanolactone

Inchi: InChI=1S/C7H12O2/c8-7-5-3-1-2-4-6-9-7/h1-6H2
InchiKey: BTLSLHNLDQCWKS-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: O=C1CCCCCCO1
Mol. weight [g/mol]: 128.17
CAS: 539-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-192.69	kJ/mol	Joback Method
hf	-411.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-465.00 ± 2.00	kJ/mol	NIST Webbook
hfus	7.94	kJ/mol	Joback Method
hvap	54.00 ± 1.00	kJ/mol	NIST Webbook
hvap	54.00	kJ/mol	NIST Webbook
hvap	53.30 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.51		Crippen Method
logp	1.494		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	487.09	K	Joback Method
tc	727.96	K	Joback Method
tf	268.02	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.72	J/mol×K	487.09	Joback Method
cpg	248.85	J/mol×K	527.23	Joback Method
cpg	265.16	J/mol×K	567.38	Joback Method
cpg	280.62	J/mol×K	607.52	Joback Method
cpg	295.20	J/mol×K	647.67	Joback Method
cpg	308.87	J/mol×K	687.81	Joback Method

cpg	321.61	J/mol×K	727.96	Joback Method
hvapt	48.20 ± 0.30	kJ/mol	379.00	NIST Webbook

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=C539877&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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/17-457-6/Heptanolactone.pdf

Generated by Cheméo on 2024-10-12 03:45:53.760315191 +0000 UTC m=+3285616.397284443.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.