

4-Ethyl-4-octanolide

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

Physical Properties

Property code	Value	Unit	Source
gf	-144.33	kJ/mol	Joback Method
hf	-443.71	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	45.72	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.662		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1359.00		NIST Webbook
rinpol	1359.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1950.00		NIST Webbook
tb	538.49	K	Joback Method
tc	751.28	K	Joback Method
tf	332.05	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.66	J/molxK	538.49	Joback Method
cpg	386.70	J/molxK	573.96	Joback Method
cpg	402.83	J/molxK	609.42	Joback Method
cpg	418.12	J/molxK	644.89	Joback Method
cpg	432.67	J/molxK	680.35	Joback Method
cpg	446.56	J/molxK	715.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R434701&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

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