ALPHA-HEXYL-GAMMA-BUTYROLACTONE

Other names: 3-hexyldihydrofuran-2(3H)-one
Inchi: InChI=1S/C10H18O2/c1-2-3-4-5-6-9-7-8-12-10(9)11/h9H,2-8H2,1H3
InchiKey: IBVDLVUXSDSVQF-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCCCCCC1CCOC1=O
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
hf	-477.74	kJ/mol	Cheméo Relay (1.0)
hfus	23.08	kJ/mol	Joback Method
hvap	67.85	kJ/mol	Cheméo Relay (1.0)
logp	2.520		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
rinpol	1441.00		NIST Webbook
tb	543.43	K	Cheméo Relay (1.0)
tf	261.24	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.23	J/mol×K	538.25	Joback Method
cpg	387.45	J/mol×K	572.33	Joback Method
cpg	403.86	J/mol×K	606.41	Joback Method
cpg	419.47	J/mol×K	640.49	Joback Method
cpg	434.30	J/mol×K	674.57	Joback Method
cpg	448.34	J/mol×K	708.65	Joback Method
cpg	461.59	J/mol×K	742.73	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18436378&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point