N-Butyryl-DL-homoserine lactone

Inchi: InChI=1S/C8H13NO3/c1-2-3-7(10)9-6-4-5-12-8(6)11/h6H,2-5H2,1H3,(H,9,10)
InchiKey: VFFNZZXXTGXBOG-UHFFFAOYSA-N
Formula: C8H13NO3
SMILES: CCCC(=O)NC1CCOC1=O
Mol. weight [g/mol]: 171.19
CAS: 98426-48-3

Physical Properties

Property code	Value	Unit	Source
gf	-195.21	kJ/mol	Joback Method
hf	-476.78	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	55.60	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	0.218		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tb	596.53	K	Joback Method
tc	815.90	K	Joback Method
tf	388.20	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.90	J/mol×K	596.53	Joback Method
cpg	360.30	J/mol×K	633.09	Joback Method
cpg	373.89	J/mol×K	669.65	Joback Method
cpg	386.67	J/mol×K	706.21	Joback Method
cpg	398.63	J/mol×K	742.78	Joback Method
cpg	409.78	J/mol×K	779.34	Joback Method
cpg	420.12	J/mol×K	815.90	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98426483&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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