

Butyric acid, 2-[(isopropylideneamino)oxy]-

Inchi:	InChI=1S/C7H13NO3/c1-4-6(7(9)10)11-8-5(2)3/h6H,4H2,1-3H3,(H,9,10)
InchiKey:	BGKAMYFJKFYFAJ-UHFFFAOYSA-N
Formula:	C7H13NO3
SMILES:	CCC(ON=C(C)C)C(=O)O
Mol. weight [g/mol]:	159.18
CAS:	5001-37-6

Physical Properties

Property code	Value	Unit	Source
hf	-517.69	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.262		Crippen Method
mcvol	128.480	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	604.15	K	Joback Method
tc	795.16	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5001376&Units=SI
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

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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