

1-Butoxypropan-2-yl nonanoate

Inchi:	InChI=1S/C16H32O3/c1-4-6-8-9-10-11-12-16(17)19-15(3)14-18-13-7-5-2/h15H,4-14H2,1
InchiKey:	DFJWSEMSFWZLQX-UHFFFAOYSA-N
Formula:	C16H32O3
SMILES:	CCCCCCCCC(=O)OC(C)COCCCC
Mol. weight [g/mol]:	272.42

Physical Properties

Property code	Value	Unit	Source
gf	-257.52	kJ/mol	Joback Method
hf	-755.87	kJ/mol	Joback Method
hfus	37.65	kJ/mol	Joback Method
hvap	62.39	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.485		Crippen Method
mcvol	249.610	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	1754.00		NIST Webbook
tb	663.75	K	Joback Method
tc	833.87	K	Joback Method
tf	349.47	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.13	J/molxK	663.75	Joback Method
cpg	789.07	J/molxK	805.52	Joback Method
cpg	774.21	J/molxK	777.17	Joback Method
cpg	758.59	J/molxK	748.81	Joback Method
cpg	742.21	J/molxK	720.46	Joback Method
cpg	725.06	J/molxK	692.10	Joback Method
cpg	803.19	J/molxK	833.87	Joback Method
dvisc	0.0000876	Paxs	663.75	Joback Method
dvisc	0.0001186	Paxs	611.37	Joback Method

dvisc	0.0001699	Paxs	558.99	Joback Method
dvisc	0.0002622	Paxs	506.61	Joback Method
dvisc	0.0004471	Paxs	454.23	Joback Method
dvisc	0.0008764	Paxs	401.85	Joback Method
dvisc	0.0021019	Paxs	349.47	Joback Method

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=U378254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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