

3-Methoxybutyl propionate

Inchi:	InChI=1S/C8H16O3/c1-4-8(9)11-6-5-7(2)10-3/h7H,4-6H2,1-3H3
InchiKey:	GHVQFNRPRTBJY-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCC(=O)OCCC(C)OC
Mol. weight [g/mol]:	160.21

Physical Properties

Property code	Value	Unit	Source
gf	-324.88	kJ/mol	Joback Method
hf	-590.75	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	44.58	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.365		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1048.00		NIST Webbook
tb	480.71	K	Joback Method
tc	658.97	K	Joback Method
tf	259.31	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.01	J/molxK	480.71	Joback Method
cpg	316.41	J/molxK	510.42	Joback Method
cpg	328.40	J/molxK	540.13	Joback Method
cpg	339.98	J/molxK	569.84	Joback Method
cpg	351.15	J/molxK	599.55	Joback Method
cpg	361.90	J/molxK	629.26	Joback Method
cpg	372.23	J/molxK	658.97	Joback Method
dvisc	0.0034290	Paxs	259.31	Joback Method
dvisc	0.0015960	Paxs	296.21	Joback Method

dvisc	0.0008800	Paxs	333.11	Joback Method
dvisc	0.0005464	Paxs	370.01	Joback Method
dvisc	0.0003699	Paxs	406.91	Joback Method
dvisc	0.0002672	Paxs	443.81	Joback Method
dvisc	0.0002029	Paxs	480.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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