

3-Methoxybutyl pentanoate

Inchi:	InChI=1S/C10H20O3/c1-4-5-6-10(11)13-8-7-9(2)12-3/h9H,4-8H2,1-3H3
InchiKey:	GAYOORNFBPOLM-UHFFFAOYSA-N
Formula:	C10H20O3
SMILES:	CCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]:	188.26

Physical Properties

Property code	Value	Unit	Source
gf	-308.04	kJ/mol	Joback Method
hf	-632.03	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.145		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1232.00		NIST Webbook
tb	526.47	K	Joback Method
tc	701.59	K	Joback Method
tf	281.85	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.46	J/molxK	526.47	Joback Method
cpg	408.75	J/molxK	555.66	Joback Method
cpg	422.52	J/molxK	584.84	Joback Method
cpg	435.78	J/molxK	614.03	Joback Method
cpg	448.52	J/molxK	643.22	Joback Method
cpg	460.74	J/molxK	672.40	Joback Method
cpg	472.44	J/molxK	701.59	Joback Method
dvisc	0.0032312	Paxs	281.85	Joback Method
dvisc	0.0014545	Paxs	322.62	Joback Method

dvisc	0.0007831	Paxs	363.39	Joback Method
dvisc	0.0004778	Paxs	404.16	Joback Method
dvisc	0.0003191	Paxs	444.93	Joback Method
dvisc	0.0002281	Paxs	485.70	Joback Method
dvisc	0.0001717	Paxs	526.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541027&Units=SI

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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