

2-Propenoic acid, 3-methoxybutyl ester

Other names:	3-Methoxybutyl acrylate
Inchi:	InChI=1S/C8H14O3/c1-4-8(9)11-6-5-7(2)10-3/h4,7H,1,5-6H2,2-3H3
InchiKey:	NPYMXLXNEYZTMQ-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	C=CC(=O)OCCC(C)OC
Mol. weight [g/mol]:	158.19
CAS:	2768-07-2

Physical Properties

Property code	Value	Unit	Source
gf	-237.04	kJ/mol	Joback Method
hf	-465.32	kJ/mol	Joback Method
hfus	15.65	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.141		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	913.00		NIST Webbook
rinpol	905.00		NIST Webbook
tb	477.39	K	Joback Method
tc	659.19	K	Joback Method
tf	257.55	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.73	J/molxK	477.39	Joback Method
cpg	298.50	J/molxK	507.69	Joback Method
cpg	309.87	J/molxK	537.99	Joback Method
cpg	320.81	J/molxK	568.29	Joback Method
cpg	331.35	J/molxK	598.59	Joback Method
cpg	341.46	J/molxK	628.89	Joback Method

cpg	351.15	J/molxK	659.19	Joback Method
dvisc	0.0031442	Paxs	257.55	Joback Method
dvisc	0.0015027	Paxs	294.19	Joback Method
dvisc	0.0008458	Paxs	330.83	Joback Method
dvisc	0.0005338	Paxs	367.47	Joback Method
dvisc	0.0003663	Paxs	404.11	Joback Method
dvisc	0.0002676	Paxs	440.75	Joback Method
dvisc	0.0002051	Paxs	477.39	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=C2768072&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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