

3-(Methoxymethoxy)butanoic acid

Inchi:	InChI=1S/C6H12O4/c1-5(3-6(7)8)10-4-9-2/h5H,3-4H2,1-2H3,(H,7,8)
InchiKey:	DGRBILULKINLRX-UHFFFAOYSA-N
Formula:	C6H12O4
SMILES:	COCOC(C)CC(=O)O
Mol. weight [g/mol]:	148.16
CAS:	1086255-73-3

Physical Properties

Property code	Value	Unit	Source
gf	-478.54	kJ/mol	Joback Method
hf	-701.70	kJ/mol	Joback Method
hfus	15.84	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.470		Crippen Method
mcvol	114.580	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
rinpol	1118.10		NIST Webbook
rinpol	1118.10		NIST Webbook
tb	527.13	K	Joback Method
tc	700.89	K	Joback Method
tf	297.59	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.80	J/mol×K	527.13	Joback Method
cpg	276.85	J/mol×K	556.09	Joback Method
cpg	285.61	J/mol×K	585.05	Joback Method
cpg	294.06	J/mol×K	614.01	Joback Method
cpg	302.20	J/mol×K	642.97	Joback Method
cpg	310.02	J/mol×K	671.93	Joback Method
cpg	317.52	J/mol×K	700.89	Joback Method

dvisc	0.0107075	Paxs	297.59	Joback Method
dvisc	0.0032396	Paxs	335.85	Joback Method
dvisc	0.0012517	Paxs	374.10	Joback Method
dvisc	0.0005769	Paxs	412.36	Joback Method
dvisc	0.0003033	Paxs	450.62	Joback Method
dvisc	0.0001763	Paxs	488.87	Joback Method
dvisc	0.0001109	Paxs	527.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1086255733&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

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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