

Methyl 3-morpholinopropionate

Inchi:	InChI=1S/C8H15NO3/c1-11-8(10)2-3-9-4-6-12-7-5-9/h2-7H2,1H3
InchiKey:	YMSLLIGKMYXCPK-UHFFFAOYSA-N
Formula:	C8H15NO3
SMILES:	COC(=O)CCN1CCOCC1
Mol. weight [g/mol]:	173.21

Physical Properties

Property code	Value	Unit	Source
af	0.5113		Cheméo Relay (1.0)
hvap	69.44	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	0.63		Cheméo Relay (1.0)
logp	-0.118		Crippen Method
mcvol	136.010	ml/mol	McGowan Method
pc	2890.30	kPa	Cheméo Relay (1.0, beta)
tb	511.52	K	Cheméo Relay (1.0)
tc	693.64	K	Cheméo Relay (1.0)
tf	265.74	K	Cheméo Relay (1.0)
vc	0.489	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33611437&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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