

Isopropyl-(2-methoxy-ethyl)-methyl-amine

Inchi:

InChI=1S/C7H17NO/c1-7(2)8(3)5-6-9-4/h7H,5-6H2,1-4H3

InchiKey:

ZFLBJYJRXLWTJI-UHFFFAOYSA-N

Formula:

C7H17NO

SMILES:

COCCN(C)C(C)C

Mol. weight [g/mol]:

131.22

Physical Properties

Property code	Value	Unit	Source
gf	11.40	kJ/mol	Joback Method
hf	-257.78	kJ/mol	Joback Method
hfus	14.57	kJ/mol	Joback Method
hvap	35.24	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	0.973		Crippen Method
mcvol	125.340	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	902.94		NIST Webbook
tb	393.98	K	Joback Method
tc	560.88	K	Joback Method
tf	208.35	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.57	J/mol×K	393.98	Joback Method
cpg	259.57	J/mol×K	421.80	Joback Method
cpg	272.12	J/mol×K	449.61	Joback Method
cpg	284.22	J/mol×K	477.43	Joback Method
cpg	295.88	J/mol×K	505.25	Joback Method
cpg	307.11	J/mol×K	533.07	Joback Method
cpg	317.92	J/mol×K	560.88	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=R513641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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