Isobutyl (3-(methylthio)propyl) carbonate

Inchi: InChI=1S/C9H18O3S/c1-8(2)7-12-9(10)11-5-4-6-13-3/h8H,4-7H2,1-3H3
InchiKey: XCCCSGSBRSRROR-UHFFFAOYSA-N
Formula: C9H18O3S
SMILES: CSCCCOC(=O)OCC(C)C
Mol. weight [g/mol]: 206.30

Physical Properties

Property code	Value	Unit	Source
gf	-283.34	kJ/mol	Joback Method
hf	-569.52	kJ/mol	Joback Method
hfus	23.65	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.549		Crippen Method
mcvol	167.330	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
tb	572.37	K	Joback Method
tc	766.49	K	Joback Method
tf	304.98	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.21	J/mol×K	572.37	Joback Method
cpg	417.13	J/mol×K	604.72	Joback Method
cpg	430.47	J/mol×K	637.08	Joback Method
cpg	443.22	J/mol×K	669.43	Joback Method
cpg	455.36	J/mol×K	701.78	Joback Method
cpg	466.87	J/mol×K	734.14	Joback Method
cpg	477.76	J/mol×K	766.49	Joback Method

Sources

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=U378275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume