N-Benzyl O-methyl thiocarbamate

Inchi: InChI=1S/C9H11NOS/c1-11-9(12)10-7-8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H,10,12)
InchiKey: HLVIWUVHOXMUET-UHFFFAOYSA-N
Formula: C9H11NOS
SMILES: COC(=S)NCc1ccccc1
Mol. weight [g/mol]: 181.25
CAS: 65263-72-1

Physical Properties

Property code	Value	Unit	Source
gf	238.76	kJ/mol	Joback Method
hf	75.19	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	53.48	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.708		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1608.00		NIST Webbook
ripol	2766.00		NIST Webbook
tb	574.63	K	Joback Method
tc	807.48	K	Joback Method
tf	326.77	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.37	J/mol×K	574.63	Joback Method
cpg	329.07	J/mol×K	613.44	Joback Method
cpg	340.85	J/mol×K	652.25	Joback Method
cpg	351.75	J/mol×K	691.05	Joback Method
cpg	361.86	J/mol×K	729.86	Joback Method
cpg	371.24	J/mol×K	768.67	Joback Method
cpg	379.94	J/mol×K	807.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65263721&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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