1-(Benzylthio)acetone

Other names:	«alpha»-(Benzylthio)acetone
	(Benzylthio)acetone
	1-(Benzylthio)-2-propanone
	2-Propanone, 1-[(phenylmethyl)thio]-
Inchi:	InChI=1S/C10H12OS/c1-9(11)7-12-8-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey:	OIEDQMIEPJIRFT-UHFFFAOYSA-N
Formula:	C10H12OS
SMILES:	CC(=O)CSCc1ccccc1
Mol. weight [g/mol]:	180.27
CAS:	10230-69-0

Physical Properties

Property code	Value	Unit	Source
gf	49.93	kJ/mol	Joback Method
hf	-83.91	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.509		Crippen Method
mcvol	145.920	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	577.53	K	Joback Method
tc	812.37	K	Joback Method
tf	313.21	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.08	J/mol×K	577.53	Joback Method
cpg	341.04	J/mol×K	616.67	Joback Method
cpg	354.04	J/mol×K	655.81	Joback Method
cpg	366.11	J/mol×K	694.95	Joback Method
cpg	377.28	J/mol×K	734.09	Joback Method

cpg	387.61	J/mol×K	773.23	Joback Method
cpg	397.11	J/mol×K	812.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10230690&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume