Benzoic acid, 3-(acetylthio)-

Inchi: InChI=1S/C9H8O3S/c1-6(10)13-8-4-2-3-7(5-8)9(11)12/h2-5H,1H3,(H,11,12)
InchiKey: CKBDDIOFRDYYFZ-UHFFFAOYSA-N
Formula: C9H8O3S
SMILES: CC(=O)Sc1cccc(C(=O)O)c1
Mol. weight [g/mol]: 196.22
CAS: 90887-44-8

Physical Properties

Property code	Value	Unit	Source
gf	-233.86	kJ/mol	Joback Method
hf	-339.55	kJ/mol	Joback Method
hfus	24.13	kJ/mol	Joback Method
hvap	75.55	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.023		Crippen Method
mcvol	139.270	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
tb	705.68	K	Joback Method
tc	932.48	K	Joback Method
tf	425.21	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.31	J/mol×K	705.68	Joback Method
cpg	343.14	J/mol×K	743.48	Joback Method
cpg	351.26	J/mol×K	781.28	Joback Method
cpg	358.70	J/mol×K	819.08	Joback Method
cpg	365.47	J/mol×K	856.88	Joback Method
cpg	371.58	J/mol×K	894.68	Joback Method
cpg	377.08	J/mol×K	932.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90887448&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

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