

Benzoic acid, 4-(acetylthio)-

Inchi:	InChI=1S/C9H8O3S/c1-6(10)13-8-4-2-7(3-5-8)9(11)12/h2-5H,1H3,(H,11,12)
InchiKey:	ZUDCIPNZEZLOLJ-UHFFFAOYSA-N
Formula:	C9H8O3S
SMILES:	CC(=O)Sc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	196.23

Physical Properties

Property code	Value	Unit	Source
af	0.6865		Cheméo Relay (1.0)
gf	-233.86	kJ/mol	Joback Method
hf	-425.33	kJ/mol	Cheméo Relay (1.0)
hfus	24.13	kJ/mol	Joback Method
hvap	99.31	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
log10ws	-2.72		Cheméo Relay (1.0)
logp	2.023		Crippen Method
mcvol	139.270	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
rinpol	1748.00		NIST Webbook
tb	579.30	K	Cheméo Relay (1.0)
tc	813.28	K	Cheméo Relay (1.0)
tf	457.70	K	Cheméo Relay (1.0)
vc	0.468	m3/kmol	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24197624&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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