Benzoic acid, 2-(acetylthio)-, methyl ester

Inchi: InChI=1S/C10H10O3S/c1-7(11)14-9-6-4-3-5-8(9)10(12)13-2/h3-6H,1-2H3
InchiKey: BNPNCJLZIHWQEF-UHFFFAOYSA-N
Formula: C10H10O3S
SMILES: COC(=O)c1ccccc1SC(C)=O
Mol. weight [g/mol]: 210.25

Physical Properties

Property code	Value	Unit	Source
gf	-193.62	kJ/mol	Joback Method
hf	-340.18	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	63.51	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.112		Crippen Method
mcvol	153.360	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1624.00		NIST Webbook
tb	658.80	K	Joback Method
tc	897.86	K	Joback Method
tf	397.89	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.90	J/mol×K	658.80	Joback Method
cpg	374.85	J/mol×K	698.64	Joback Method
cpg	385.92	J/mol×K	738.49	Joback Method
cpg	396.11	J/mol×K	778.33	Joback Method
cpg	405.42	J/mol×K	818.17	Joback Method
cpg	413.85	J/mol×K	858.01	Joback Method
cpg	421.40	J/mol×K	897.86	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=U375164&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume