S-benzylthioacetate

Inchi: InChI=1S/C9H10OS/c1-8(10)11-7-9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey: XQLIUJWBXPIGCB-UHFFFAOYSA-N
Formula: C9H10OS
SMILES: CC(=O)SCc1ccccc1
Mol. weight [g/mol]: 166.24

Physical Properties

Property code	Value	Unit	Source
gf	41.51	kJ/mol	Joback Method
hf	-63.27	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	51.47	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.466		Crippen Method
mcvol	131.830	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
ripol	1986.00		NIST Webbook
ripol	1986.00		NIST Webbook
tb	554.65	K	Joback Method
tc	794.33	K	Joback Method
tf	301.94	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.39	J/mol×K	554.65	Joback Method
cpg	294.44	J/mol×K	594.60	Joback Method
cpg	306.58	J/mol×K	634.54	Joback Method
cpg	317.84	J/mol×K	674.49	Joback Method
cpg	328.25	J/mol×K	714.43	Joback Method
cpg	337.83	J/mol×K	754.38	Joback Method
cpg	346.63	J/mol×K	794.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R336479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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