Benzoic acid, 3-(methylthio)-

Inchi: InChI=1S/C8H8O2S/c1-11-7-4-2-3-6(5-7)8(9)10/h2-5H,1H3,(H,9,10)
InchiKey: PZGADOOBMVLBJE-UHFFFAOYSA-N
Formula: C8H8O2S
SMILES: CSc1cccc(C(=O)O)c1
Mol. weight [g/mol]: 168.21
CAS: 825-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-113.36	kJ/mol	Joback Method
hf	-206.33	kJ/mol	Joback Method
hfus	19.95	kJ/mol	Joback Method
hvap	66.58	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.107		Crippen Method
mcvol	123.610	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
tb	628.93	K	Joback Method
tc	853.69	K	Joback Method
tf	364.01	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.94	J/mol×K	628.93	Joback Method
cpg	288.27	J/mol×K	666.39	Joback Method
cpg	296.94	J/mol×K	703.85	Joback Method
cpg	304.99	J/mol×K	741.31	Joback Method
cpg	312.42	J/mol×K	778.77	Joback Method
cpg	319.25	J/mol×K	816.23	Joback Method
cpg	325.51	J/mol×K	853.69	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=C825990&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

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