

Benzoic acid, 3-(ethylthio)-, ethyl ester

Inchi:	InChI=1S/C11H14O2S/c1-3-13-11(12)9-6-5-7-10(8-9)14-4-2/h5-8H,3-4H2,1-2H3
InchiKey:	CFYKQXZGVYROJJ-UHFFFAOYSA-N
Formula:	C11H14O2S
SMILES:	CCOC(=O)c1cccc(SCC)c1
Mol. weight [g/mol]:	210.29

Physical Properties

Property code	Value	Unit	Source
gf	-56.28	kJ/mol	Joback Method
hf	-248.24	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	58.99	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.975		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinqol	1661.00		NIST Webbook
tb	627.81	K	Joback Method
tc	855.76	K	Joback Method
tf	359.23	K	Joback Method
vc	0.622	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.30	J/molxK	627.81	Joback Method
cpg	412.46	J/molxK	665.80	Joback Method
cpg	425.72	J/molxK	703.79	Joback Method
cpg	438.10	J/molxK	741.78	Joback Method
cpg	449.59	J/molxK	779.77	Joback Method
cpg	460.21	J/molxK	817.77	Joback Method
cpg	469.97	J/molxK	855.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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