

Benzoic acid, 3-(methylthio)-, pentyl ester

Inchi:	InChI=1S/C13H18O2S/c1-3-4-5-9-15-13(14)11-7-6-8-12(10-11)16-2/h6-8,10H,3-5,9H2,1
InchiKey:	BVKWZQWWQWGYTH-UHFFFAOYSA-N
Formula:	C13H18O2S
SMILES:	CCCCCOC(=O)c1cccc(SC)c1
Mol. weight [g/mol]:	238.35

Physical Properties

Property code	Value	Unit	Source
gf	-39.44	kJ/mol	Joback Method
hf	-289.52	kJ/mol	Joback Method
hfus	29.99	kJ/mol	Joback Method
hvap	63.44	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.756		Crippen Method
mvol	194.060	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
tb	673.57	K	Joback Method
tc	893.32	K	Joback Method
tf	381.77	K	Joback Method
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.32	J/molxK	673.57	Joback Method
cpg	514.64	J/molxK	710.20	Joback Method
cpg	528.98	J/molxK	746.82	Joback Method
cpg	542.35	J/molxK	783.45	Joback Method
cpg	554.78	J/molxK	820.07	Joback Method
cpg	566.27	J/molxK	856.70	Joback Method
cpg	576.85	J/molxK	893.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374946&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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