Benzoic acid, 2-(pentylthio)-

Inchi: InChI=1S/C12H16O2S/c1-2-3-6-9-14-12(13)10-7-4-5-8-11(10)15/h4-5,7-8,15H,2-3,6,9H2
InchiKey: GWKVYTATPQASGX-UHFFFAOYSA-N
Formula: C12H16O2S
SMILES: CCCCCOC(=O)c1ccccc1S
Mol. weight [g/mol]: 224.32

Physical Properties

Property code	Value	Unit	Source
gf	-51.59	kJ/mol	Joback Method
hf	-272.27	kJ/mol	Joback Method
hfus	27.32	kJ/mol	Joback Method
hvap	61.14	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.322		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1956.00		NIST Webbook
tb	644.77	K	Joback Method
tc	868.96	K	Joback Method
tf	372.56	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.03	J/mol×K	644.77	Joback Method
cpg	459.77	J/mol×K	682.13	Joback Method
cpg	473.58	J/mol×K	719.50	Joback Method
cpg	486.47	J/mol×K	756.86	Joback Method
cpg	498.48	J/mol×K	794.23	Joback Method
cpg	509.62	J/mol×K	831.59	Joback Method
cpg	519.93	J/mol×K	868.96	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=U374976&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