Benzoic acid, 2-(propylthio)-, propyl ester

Inchi: InChI=1S/C13H18O2S/c1-3-9-15-13(14)11-7-5-6-8-12(11)16-10-4-2/h5-8H,3-4,9-10H2,1
InchiKey: VNNNMTQMWUZREH-UHFFFAOYSA-N
Formula: C13H18O2S
SMILES: CCCOC(=O)c1ccccc1SCCC
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
mcvol	194.060	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1823.00		NIST Webbook
tb	673.57	K	Joback Method
tc	893.32	K	Joback Method
tf	381.77	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.32	J/mol×K	673.57	Joback Method
cpg	514.64	J/mol×K	710.20	Joback Method
cpg	528.98	J/mol×K	746.82	Joback Method
cpg	542.35	J/mol×K	783.45	Joback Method
cpg	554.78	J/mol×K	820.07	Joback Method
cpg	566.27	J/mol×K	856.70	Joback Method
cpg	576.85	J/mol×K	893.32	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=U374972&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume