Benzoic acid, 2-(pentylthio)-, pentyl ester

Inchi: InChI=1S/C17H26O2S/c1-3-5-9-13-19-17(18)15-11-7-8-12-16(15)20-14-10-6-4-2/h7-8,11
InchiKey: UIJRCGNNUGIBRI-UHFFFAOYSA-N
Formula: C17H26O2S
SMILES: CCCCCOC(=O)c1ccccc1SCCCCC
Mol. weight [g/mol]: 294.45

Physical Properties

Property code	Value	Unit	Source
gf	-5.76	kJ/mol	Joback Method
hf	-372.08	kJ/mol	Joback Method
hfus	40.35	kJ/mol	Joback Method
hvap	72.35	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.316		Crippen Method
mcvol	250.420	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	765.09	K	Joback Method
tc	973.17	K	Joback Method
tf	426.85	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.81	J/mol×K	765.09	Joback Method
cpg	733.45	J/mol×K	799.77	Joback Method
cpg	749.00	J/mol×K	834.45	Joback Method
cpg	763.48	J/mol×K	869.13	Joback Method
cpg	776.91	J/mol×K	903.81	Joback Method
cpg	789.33	J/mol×K	938.49	Joback Method
cpg	800.75	J/mol×K	973.17	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=U374973&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