Benzoic acid, 4-(butylthio)-, butyl ester

Inchi: InChI=1S/C15H22O2S/c1-3-5-11-17-15(16)13-7-9-14(10-8-13)18-12-6-4-2/h7-10H,3-6,1
InchiKey: CPRYHODEDAKYRR-UHFFFAOYSA-N
Formula: C15H22O2S
SMILES: CCCCOC(=O)c1ccc(SCCCC)cc1
Mol. weight [g/mol]: 266.40

Physical Properties

Property code	Value	Unit	Source
gf	-22.60	kJ/mol	Joback Method
hf	-330.80	kJ/mol	Joback Method
hfus	35.17	kJ/mol	Joback Method
hvap	67.90	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.536		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2119.00		NIST Webbook
rinpol	2119.00		NIST Webbook
tb	719.33	K	Joback Method
tc	932.35	K	Joback Method
tf	404.31	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.72	J/mol×K	719.33	Joback Method
cpg	621.83	J/mol×K	754.83	Joback Method
cpg	636.90	J/mol×K	790.34	Joback Method
cpg	650.95	J/mol×K	825.84	Joback Method
cpg	663.99	J/mol×K	861.34	Joback Method
cpg	676.06	J/mol×K	896.85	Joback Method
cpg	687.16	J/mol×K	932.35	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=U374964&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