Benzoic acid, 2-(butylthio)-

Inchi: InChI=1S/C11H14O2S/c1-2-3-8-13-11(12)9-6-4-5-7-10(9)14/h4-7,14H,2-3,8H2,1H3
InchiKey: UOTKBRDRSXAZOM-UHFFFAOYSA-N
Formula: C11H14O2S
SMILES: CCCCOC(=O)c1ccccc1S
Mol. weight [g/mol]: 210.29

Physical Properties

Property code	Value	Unit	Source
gf	-60.01	kJ/mol	Joback Method
hf	-251.63	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	58.91	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.932		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1856.00		NIST Webbook
rinpol	1856.00		NIST Webbook
tb	621.89	K	Joback Method
tc	850.38	K	Joback Method
tf	361.29	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.54	J/mol×K	621.89	Joback Method
cpg	409.62	J/mol×K	659.97	Joback Method
cpg	422.82	J/mol×K	698.05	Joback Method
cpg	435.14	J/mol×K	736.13	Joback Method
cpg	446.60	J/mol×K	774.22	Joback Method
cpg	457.23	J/mol×K	812.30	Joback Method
cpg	467.05	J/mol×K	850.38	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=U374977&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