Thiobenzoic acid, S-n-butyl ester

Other names:	n-Butylthio benzoate
	Butyl thiobenzoate
	Benzenecarbothioic acid, S-butyl ester
	Benzoic acid, thio-, S-butyl ester
	Thiobenzoic acid S-butyl ester
	S-Butyl thiobenzoate
	Butyl thiolbenzoate
	S-Butyl benzenecarbothioate
Inchi:	InChI=1S/C11H14OS/c1-2-3-9-13-11(12)10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3
InchiKey:	KXXZPIFZTPWOJJ-UHFFFAOYSA-N
Formula:	C11H14OS
SMILES:	CCCCSC(=O)c1ccccc1
Mol. weight [g/mol]:	194.29
CAS:	7269-35-4

Physical Properties

Property code	Value	Unit	Source
gf	58.35	kJ/mol	Joback Method
hf	-104.55	kJ/mol	Joback Method
hfus	24.02	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.360		Crippen Method
mcvol	160.010	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1640.00		NIST Webbook
tb	600.41	K	Joback Method
tc	830.60	K	Joback Method
tf	324.48	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	374.46	J/mol×K	600.41	Joback Method
cpg	389.18	J/mol×K	638.77	Joback Method
cpg	402.90	J/mol×K	677.14	Joback Method
cpg	415.66	J/mol×K	715.50	Joback Method
cpg	427.50	J/mol×K	753.87	Joback Method
cpg	438.45	J/mol×K	792.23	Joback Method
cpg	448.55	J/mol×K	830.60	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C7269354&Units=SI

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