Hexanoic acid, thio-, S-butyl ester

Other names: S-Butylthiohexanoate
Inchi: InChI=1S/C10H20OS/c1-3-5-7-8-10(11)12-9-6-4-2/h3-9H2,1-2H3
InchiKey: FBORYKJGJUDLQA-UHFFFAOYSA-N
Formula: C10H20OS
SMILES: CCCCCC(=O)SCCCC
Mol. weight [g/mol]: 188.33
CAS: 2432-79-3

Physical Properties

Property code	Value	Unit	Source
gf	-62.48	kJ/mol	Joback Method
hf	-320.44	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.627		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
ripol	1607.00		NIST Webbook
ripol	1609.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1609.00		NIST Webbook
tb	550.85	K	Joback Method
tc	741.62	K	Joback Method
tf	286.79	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.59	J/mol×K	550.85	Joback Method
cpg	414.40	J/mol×K	582.64	Joback Method
cpg	428.53	J/mol×K	614.44	Joback Method
cpg	442.00	J/mol×K	646.23	Joback Method

cpg	454.81	J/mol×K	678.03	Joback Method
cpg	466.98	J/mol×K	709.82	Joback Method
cpg	478.53	J/mol×K	741.62	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=C2432793&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume