

Butyl tert-butyl sulfide

Other names:	tert-Butyl butyl sulfide
Inchi:	InChI=1S/C8H18S/c1-5-6-7-9-8(2,3)4/h5-7H2,1-4H3
InchiKey:	XRYKNXGXIFPTKH-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CCCCSC(C)(C)C
Mol. weight [g/mol]:	146.29
CAS:	926-47-6

Physical Properties

Property code	Value	Unit	Source
gf	52.44	kJ/mol	Joback Method
hf	-175.33	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	38.92	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.318		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
tb	447.99	K	Joback Method
tc	645.76	K	Joback Method
tf	216.74	K	Joback Method
vc	0.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.36	J/mol×K	447.99	Joback Method
cpg	304.61	J/mol×K	480.95	Joback Method
cpg	319.08	J/mol×K	513.91	Joback Method
cpg	332.81	J/mol×K	546.87	Joback Method

cpg	345.81	J/mol×K	579.83	Joback Method
cpg	358.11	J/mol×K	612.79	Joback Method
cpg	369.75	J/mol×K	645.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C926476&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
mvol:	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

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