

Butyl furfuryl sulfide

Inchi:	InChI=1S/C10H16S/c1-2-3-8-11-9-10-6-4-5-7-10/h4-6H,2-3,7-9H2,1H3
InchiKey:	GUIUGOUTYXUIJV-UHFFFAOYSA-N
Formula:	C10H16S
SMILES:	CCCCSCC1=CC=CC1
Mol. weight [g/mol]:	168.30

Physical Properties

Property code	Value	Unit	Source
gf	160.99	kJ/mol	Joback Method
hf	-22.95	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	46.48	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.406		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1248.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1256.00		NIST Webbook
tb	520.23	K	Joback Method
tc	736.26	K	Joback Method
tf	266.04	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.35	J/mol×K	520.23	Joback Method
cpg	343.02	J/mol×K	556.24	Joback Method
cpg	357.78	J/mol×K	592.24	Joback Method

cpg	371.67	J/mol×K	628.25	Joback Method
cpg	384.72	J/mol×K	664.25	Joback Method
cpg	396.97	J/mol×K	700.26	Joback Method
cpg	408.46	J/mol×K	736.26	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=R43855&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

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