Disulfide, butyl (1-methylethyl)

Other names:	Isopropyl n-butyl disulphide
	2-methyl-3,4-dithiaoctane
Inchi:	InChI=1S/C7H16S2/c1-4-5-6-8-9-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	HODYAASMHKKQBS-UHFFFAOYSA-N
Formula:	C7H16S2
SMILES:	CCCCSSC(C)C
Mol. weight [g/mol]:	164.33
CAS:	72437-53-7

Physical Properties

Property code	Value	Unit	Source
gf	71.86	kJ/mol	Joback Method
hf	-109.35	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	44.42	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.576		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1163.00		NIST Webbook
ripol	1445.00		NIST Webbook
tb	496.68	K	Joback Method
tc	710.61	K	Joback Method
tf	222.45	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.60	J/mol×K	496.68	Joback Method
cpg	310.45	J/mol×K	532.33	Joback Method
cpg	323.66	J/mol×K	567.99	Joback Method

cpg	336.24	J/mol×K	603.64	Joback Method
cpg	348.17	J/mol×K	639.30	Joback Method
cpg	359.48	J/mol×K	674.95	Joback Method
cpg	370.16	J/mol×K	710.61	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=C72437537&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume