

n-Propyl sec-butyl disulfide

Other names:	Disulfide, 1-methylpropyl propyl 3-Methyl-4,5-dithiaoctane sec-Butyl propyl disulfide 1-Propyl sec-butyl disulfide
Inchi:	InChI=1S/C7H16S2/c1-4-6-8-9-7(3)5-2/h7H,4-6H2,1-3H3
InchiKey:	KHTNPVYWCGRQEA-UHFFFAOYSA-N
Formula:	C7H16S2
SMILES:	CCCSSC(C)CC
Mol. weight [g/mol]:	164.33
CAS:	59849-54-6

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	1172.00		NIST Webbook
rinpol	1169.20		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1166.00		NIST Webbook
ripol	1448.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59849546&Units=SI
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

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
mccvol:	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

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