

8-methyl-4,5-dithia-1-nonene

Inchi:	InChI=1S/C8H16S2/c1-4-6-9-10-7-5-8(2)3/h4,8H,1,5-7H2,2-3H3
InchiKey:	GOWDCBYGCIQZTR-UHFFFAOYSA-N
Formula:	C8H16S2
SMILES:	C=CCSSCCC(C)C
Mol. weight [g/mol]:	176.34

Physical Properties

Property code	Value	Unit	Source
gf	168.12	kJ/mol	Joback Method
hf	-4.56	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.600		Crippen Method
mcvol	151.980	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1246.00		NIST Webbook
tb	516.24	K	Joback Method
tc	731.44	K	Joback Method
tf	231.96	K	Joback Method
vc	0.567	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.52	J/mol×K	516.24	Joback Method
cpg	336.72	J/mol×K	552.11	Joback Method
cpg	350.21	J/mol×K	587.97	Joback Method
cpg	362.98	J/mol×K	623.84	Joback Method
cpg	375.06	J/mol×K	659.71	Joback Method
cpg	386.44	J/mol×K	695.57	Joback Method
cpg	397.16	J/mol×K	731.44	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=R157687&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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