2,6-dithiaoctane

Inchi: InChI=1S/C6H14S2/c1-3-8-6-4-5-7-2/h3-6H2,1-2H3
InchiKey: HNTGKDAWTFWBBI-UHFFFAOYSA-N
Formula: C6H14S2
SMILES: CCSCCCSC
Mol. weight [g/mol]: 150.31

Physical Properties

Property code	Value	Unit	Source
gf	65.88	kJ/mol	Joback Method
hf	-83.43	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	42.58	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.493		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1202.00		NIST Webbook
rinpol	1202.00		NIST Webbook
tb	474.24	K	Joback Method
tc	686.46	K	Joback Method
tf	226.18	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.01	J/mol×K	474.24	Joback Method
cpg	266.31	J/mol×K	509.61	Joback Method
cpg	278.07	J/mol×K	544.98	Joback Method
cpg	289.29	J/mol×K	580.35	Joback Method
cpg	299.98	J/mol×K	615.72	Joback Method
cpg	310.13	J/mol×K	651.09	Joback Method
cpg	319.76	J/mol×K	686.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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