4-methyl-3,5-dithia-7-octene

Inchi: InChI=1S/C7H14S2/c1-4-6-9-7(3)8-5-2/h4,7H,1,5-6H2,2-3H3
InchiKey: WVOPPLMBKYMZSE-UHFFFAOYSA-N
Formula: C7H14S2
SMILES: C=CCSC(C)SCC
Mol. weight [g/mol]: 162.32

Physical Properties

Property code	Value	Unit	Source
gf	159.70	kJ/mol	Joback Method
hf	16.08	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	43.75	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	3.005		Crippen Method
mcvol	137.890	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1155.00		NIST Webbook
rinpol	1155.00		NIST Webbook
tb	493.36	K	Joback Method
tc	712.09	K	Joback Method
tf	220.69	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.92	J/mol×K	493.36	Joback Method
cpg	292.06	J/mol×K	529.82	Joback Method
cpg	304.53	J/mol×K	566.27	Joback Method
cpg	316.35	J/mol×K	602.73	Joback Method
cpg	327.54	J/mol×K	639.18	Joback Method
cpg	338.08	J/mol×K	675.64	Joback Method
cpg	348.01	J/mol×K	712.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157107&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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