5-methyl-4,7-dithia-1,9-decadiene

Inchi: InChI=1S/C9H16S2/c1-4-6-10-8-9(3)11-7-5-2/h4-5,9H,1-2,6-8H2,3H3
InchiKey: ALRSWITZDHDTPH-UHFFFAOYSA-N
Formula: C9H16S2
SMILES: C=CCSCC(C)SCC=C
Mol. weight [g/mol]: 188.35

Physical Properties

Property code	Value	Unit	Source
gf	264.38	kJ/mol	Joback Method
hf	100.23	kJ/mol	Joback Method
hfus	21.24	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.213		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1367.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1871.00		NIST Webbook
tb	535.80	K	Joback Method
tc	752.09	K	Joback Method
tf	241.47	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.94	J/mol×K	535.80	Joback Method
cpg	363.41	J/mol×K	571.85	Joback Method
cpg	377.09	J/mol×K	607.90	Joback Method
cpg	389.99	J/mol×K	643.95	Joback Method
cpg	402.14	J/mol×K	679.99	Joback Method
cpg	413.55	J/mol×K	716.04	Joback Method
cpg	424.26	J/mol×K	752.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225720&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume