4,7-Diethyl-1,2,3,5,6-pentathiepane

Inchi: InChI=1S/C6H12S5/c1-3-5-7-8-6(4-2)10-11-9-5/h5-6H,3-4H2,1-2H3
InchiKey: XOMXUEDCMMCZIK-UHFFFAOYSA-N
Formula: C6H12S5
SMILES: CCC1SSSC(CC)SS1
Mol. weight [g/mol]: 244.48
CAS: 878997-71-8

Physical Properties

Property code	Value	Unit	Source
gf	203.58	kJ/mol	Joback Method
hf	86.95	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.883		Crippen Method
mcvol	166.290	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
rinpol	1897.30		NIST Webbook
rinpol	1897.30		NIST Webbook
tb	594.98	K	Joback Method
tc	887.47	K	Joback Method
tf	574.25	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.09	J/mol×K	594.98	Joback Method
cpg	372.23	J/mol×K	643.73	Joback Method
cpg	387.10	J/mol×K	692.48	Joback Method
cpg	400.74	J/mol×K	741.22	Joback Method
cpg	413.18	J/mol×K	789.97	Joback Method
cpg	424.46	J/mol×K	838.72	Joback Method
cpg	434.63	J/mol×K	887.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C878997718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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