

5-ethyl-2,3,4,6-tetrathiaheptane

Inchi:	InChI=1S/C5H12S4/c1-4-5(6-2)8-9-7-3/h5H,4H2,1-3H3
InchiKey:	FLXQNPJSNNWYNL-UHFFFAOYSA-N
Formula:	C5H12S4
SMILES:	CCC(SC)SSSC
Mol. weight [g/mol]:	200.41
CAS:	126876-25-3

Physical Properties

Property code	Value	Unit	Source
gf	121.26	kJ/mol	Joback Method
hf	15.67	kJ/mol	Joback Method
hfus	21.70	kJ/mol	Joback Method
hvap	53.60	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.745		Crippen Method
mcvol	146.710	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	1452.00		NIST Webbook
rinpol	1483.60		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1483.60		NIST Webbook
rinpol	1452.00		NIST Webbook
tb	588.48	K	Joback Method
tc	853.93	K	Joback Method
tf	268.71	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.99	J/molxK	588.48	Joback Method
cpg	315.45	J/molxK	632.72	Joback Method
cpg	327.09	J/molxK	676.96	Joback Method
cpg	337.88	J/molxK	721.21	Joback Method

cpg	347.78	J/mol×K	765.45	Joback Method
cpg	356.77	J/mol×K	809.69	Joback Method
cpg	364.80	J/mol×K	853.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C126876253&Units=SI

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
mvol:	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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