6-Ethyl-4,5,7,8-tetrathiaundecane

Inchi: InChI=1S/C9H20S4/c1-4-7-10-12-9(6-3)13-11-8-5-2/h9H,4-8H2,1-3H3
InchiKey: RIOBTICKNGDVHT-UHFFFAOYSA-N
Formula: C9H20S4
SMILES: CCCSSC(CC)SSCCC
Mol. weight [g/mol]: 256.51
CAS: 126876-35-5

Physical Properties

Property code	Value	Unit	Source
gf	154.94	kJ/mol	Joback Method
hf	-66.89	kJ/mol	Joback Method
hfus	32.06	kJ/mol	Joback Method
hvap	62.51	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.305		Crippen Method
mcvol	203.070	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1744.40		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1799.60		NIST Webbook
rinpol	1744.40		NIST Webbook
rinpol	1799.60		NIST Webbook
tb	680.00	K	Joback Method
tc	922.09	K	Joback Method
tf	313.79	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.97	J/mol×K	680.00	Joback Method
cpg	512.66	J/mol×K	720.35	Joback Method
cpg	527.23	J/mol×K	760.70	Joback Method
cpg	540.69	J/mol×K	801.05	Joback Method

cpg	553.03	J/mol×K	841.40	Joback Method
cpg	564.24	J/mol×K	881.75	Joback Method
cpg	574.31	J/mol×K	922.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126876355&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