6-methyl-4-thiaundecane

Inchi: InChI=1S/C11H24S/c1-4-6-7-8-11(3)10-12-9-5-2/h11H,4-10H2,1-3H3
InchiKey: HSJWPFRQUVKUQP-UHFFFAOYSA-N
Formula: C11H24S
SMILES: CCCCCC(C)CSCCC
Mol. weight [g/mol]: 188.37

Physical Properties

Property code	Value	Unit	Source
gf	72.42	kJ/mol	Joback Method
hf	-233.78	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	46.51	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	4.346		Crippen Method
mcvol	182.200	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1301.00		NIST Webbook
rinpol	1301.00		NIST Webbook
tb	519.42	K	Joback Method
tc	703.22	K	Joback Method
tf	233.13	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.55	J/mol×K	519.42	Joback Method
cpg	440.48	J/mol×K	550.05	Joback Method
cpg	456.69	J/mol×K	580.69	Joback Method
cpg	472.19	J/mol×K	611.32	Joback Method
cpg	487.00	J/mol×K	641.95	Joback Method
cpg	501.13	J/mol×K	672.59	Joback Method
cpg	514.59	J/mol×K	703.22	Joback Method

Sources

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=R157607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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