3,3,5,5-tetramethyl-4-thiaheptane

Inchi: InChI=1S/C10H22S/c1-7-9(3,4)11-10(5,6)8-2/h7-8H2,1-6H3
InchiKey: UXIURYRDRSUHPC-UHFFFAOYSA-N
Formula: C10H22S
SMILES: CCC(C)(C)SC(C)(C)CC
Mol. weight [g/mol]: 174.35

Physical Properties

Property code	Value	Unit	Source
gf	72.12	kJ/mol	Joback Method
hf	-225.36	kJ/mol	Joback Method
hfus	10.96	kJ/mol	Joback Method
hvap	42.08	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.097		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	1121.00		NIST Webbook
tb	490.52	K	Joback Method
tc	696.05	K	Joback Method
tf	241.70	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.30	J/mol×K	490.52	Joback Method
cpg	399.70	J/mol×K	524.78	Joback Method
cpg	416.99	J/mol×K	559.03	Joback Method
cpg	433.22	J/mol×K	593.29	Joback Method
cpg	448.46	J/mol×K	627.54	Joback Method
cpg	462.76	J/mol×K	661.80	Joback Method
cpg	476.17	J/mol×K	696.05	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=R156406&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