2,3,5,6-tetramethyl-4-thiaheptane

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

Physical Properties

Property code	Value	Unit	Source
gf	56.68	kJ/mol	Joback Method
hf	-228.98	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	43.12	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.809		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
tb	495.22	K	Joback Method
tc	693.44	K	Joback Method
tf	176.86	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.62	J/mol×K	495.22	Joback Method
cpg	394.10	J/mol×K	528.26	Joback Method
cpg	410.77	J/mol×K	561.29	Joback Method
cpg	426.65	J/mol×K	594.33	Joback Method
cpg	441.76	J/mol×K	627.37	Joback Method
cpg	456.12	J/mol×K	660.40	Joback Method
cpg	469.74	J/mol×K	693.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155463&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
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