2,6,6-trimethyl-5-thiaoctane

Inchi: InChI=1S/C10H22S/c1-6-10(4,5)11-8-7-9(2)3/h9H,6-8H2,1-5H3
InchiKey: YQDDWNNQOGRJJP-UHFFFAOYSA-N
Formula: C10H22S
SMILES: CCC(C)(C)SCCC(C)C
Mol. weight [g/mol]: 174.35

Physical Properties

Property code	Value	Unit	Source
gf	66.84	kJ/mol	Joback Method
hf	-221.89	kJ/mol	Joback Method
hfus	14.85	kJ/mol	Joback Method
hvap	42.99	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.954		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
tb	493.31	K	Joback Method
tc	690.70	K	Joback Method
tf	224.28	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.81	J/mol×K	493.31	Joback Method
cpg	396.27	J/mol×K	526.21	Joback Method
cpg	412.82	J/mol×K	559.11	Joback Method
cpg	428.50	J/mol×K	592.01	Joback Method
cpg	443.35	J/mol×K	624.91	Joback Method
cpg	457.39	J/mol×K	657.80	Joback Method
cpg	470.67	J/mol×K	690.70	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=R155809&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