S-methylthiodecanoate

Inchi: InChI=1S/C11H22OS/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3-10H2,1-2H3
InchiKey: ZEBQAJHDEMWJOU-UHFFFAOYSA-N
Formula: C11H22OS
SMILES: CCCCCCCCCC(=O)SC
Mol. weight [g/mol]: 202.36

Physical Properties

Property code	Value	Unit	Source
gf	-54.06	kJ/mol	Joback Method
hf	-341.08	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	53.64	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.017		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
tb	573.73	K	Joback Method
tc	762.23	K	Joback Method
tf	298.06	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.25	J/mol×K	573.73	Joback Method
cpg	463.77	J/mol×K	605.15	Joback Method
cpg	478.56	J/mol×K	636.56	Joback Method
cpg	492.65	J/mol×K	667.98	Joback Method
cpg	506.06	J/mol×K	699.40	Joback Method
cpg	518.78	J/mol×K	730.82	Joback Method
cpg	530.85	J/mol×K	762.23	Joback Method

Sources

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=R237659&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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