3-(methylthio)propyl hexanoate

Inchi: InChI=1S/C10H20O2S/c1-3-4-5-7-10(11)12-8-6-9-13-2/h3-9H2,1-2H3
InchiKey: NZDCNAMVIRTJPL-UHFFFAOYSA-N
Formula: C10H20O2S
SMILES: CCCCCC(=O)OCCCSC
Mol. weight [g/mol]: 204.33

Physical Properties

Property code	Value	Unit	Source
gf	-167.48	kJ/mol	Joback Method
hf	-452.66	kJ/mol	Joback Method
hfus	28.57	kJ/mol	Joback Method
hvap	53.83	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.863		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
ripol	1973.00		NIST Webbook
tb	573.27	K	Joback Method
tc	762.70	K	Joback Method
tf	309.02	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.53	J/mol×K	573.27	Joback Method
cpg	440.09	J/mol×K	604.84	Joback Method
cpg	454.02	J/mol×K	636.41	Joback Method
cpg	467.31	J/mol×K	667.99	Joback Method
cpg	479.97	J/mol×K	699.56	Joback Method
cpg	492.00	J/mol×K	731.13	Joback Method
cpg	503.40	J/mol×K	762.70	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=R327123&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume