hexyl 3-(methylthio)propanoate

Inchi: InChI=1S/C10H20O2S/c1-4-6-9(13-3)7-8-12-10(11)5-2/h9H,4-8H2,1-3H3
InchiKey: LRZFIJCVXUBBRY-UHFFFAOYSA-N
Formula: C10H20O2S
SMILES: CCCC(CCOC(=O)CC)SC
Mol. weight [g/mol]: 204.33

Physical Properties

Property code	Value	Unit	Source
gf	-169.92	kJ/mol	Joback Method
hf	-457.94	kJ/mol	Joback Method
hfus	25.05	kJ/mol	Joback Method
hvap	53.44	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.861		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
ripol	1958.00		NIST Webbook
ripol	1958.00		NIST Webbook
tb	572.83	K	Joback Method
tc	765.97	K	Joback Method
tf	294.02	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.88	J/mol×K	572.83	Joback Method
cpg	440.79	J/mol×K	605.02	Joback Method
cpg	455.03	J/mol×K	637.21	Joback Method
cpg	468.59	J/mol×K	669.40	Joback Method
cpg	481.49	J/mol×K	701.59	Joback Method
cpg	493.72	J/mol×K	733.78	Joback Method
cpg	505.29	J/mol×K	765.97	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=R327301&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume