

2-[(methylthio)methyl]-5-(methylthio)-2-pentenal

Inchi:	InChI=1S/C8H14OS2/c1-10-5-3-4-8(6-9)7-11-2/h4,6H,3,5,7H2,1-2H3/b8-4+
InchiKey:	VVZWQNGEMWJSTM-XBXARRHUSA-N
Formula:	C8H14OS2
SMILES:	CSCCC=C(C=O)CSC
Mol. weight [g/mol]:	190.33

Physical Properties

Property code	Value	Unit	Source
gf	54.87	kJ/mol	Joback Method
hf	-102.86	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	53.79	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.228		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
tb	572.70	K	Joback Method
tc	795.53	K	Joback Method
tf	271.68	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.91	J/molxK	572.70	Joback Method
cpg	352.60	J/molxK	609.84	Joback Method
cpg	364.54	J/molxK	646.98	Joback Method
cpg	375.76	J/molxK	684.11	Joback Method
cpg	386.27	J/molxK	721.25	Joback Method
cpg	396.11	J/molxK	758.39	Joback Method
cpg	405.29	J/molxK	795.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U366011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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