

3-(Acetylthio)-2-pentylnonanal

Inchi:	InChI=1S/C16H30O2S/c1-4-6-8-10-12-16(19-14(3)18)15(13-17)11-9-7-5-2/h13,15-16H,4
InchiKey:	SUJPNFCSTIZIQF-UHFFFAOYSA-N
Formula:	C16H30O2S
SMILES:	CCCCCCC(SC(C)=O)C(C=O)CCCCC
Mol. weight [g/mol]:	286.47

Physical Properties

Property code	Value	Unit	Source
gf	-116.36	kJ/mol	Joback Method
hf	-540.42	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	70.72	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	5.001		Crippen Method
mcvol	255.790	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
ripol	1917.00		NIST Webbook
ripol	1909.00		NIST Webbook
ripol	1917.00		NIST Webbook
ripol	2436.00		NIST Webbook
ripol	2449.00		NIST Webbook
ripol	2449.00		NIST Webbook
tb	735.91	K	Joback Method
tc	926.31	K	Joback Method
tf	366.41	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.26	J/molxK	735.91	Joback Method
cpg	756.07	J/molxK	767.64	Joback Method
cpg	771.94	J/molxK	799.38	Joback Method
cpg	786.89	J/molxK	831.11	Joback Method

cpg	800.96	J/mol×K	862.84	Joback Method
cpg	814.17	J/mol×K	894.57	Joback Method
cpg	826.56	J/mol×K	926.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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