

3-(Acetylthio)-2-propylheptanal

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H22O2S/c1-4-6-8-12(15-10(3)14)11(9-13)7-5-2/h9,11-12H,4-8H2,1-3H3

LQLZAAWYPGNZTR-UHFFFAOYSA-N

C12H22O2S

CCCCC(SC(C)=O)C(C=O)CCC

230.37

Physical Properties

Property code	Value	Unit	Source
gf	-150.04	kJ/mol	Joback Method
hf	-457.86	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	61.81	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.440		Crippen Method
mcvol	199.430	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
ripol	2087.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2087.00		NIST Webbook
tb	644.39	K	Joback Method
tc	841.09	K	Joback Method
tf	321.33	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.68	J/mol×K	644.39	Joback Method
cpg	536.90	J/mol×K	677.17	Joback Method
cpg	551.30	J/mol×K	709.96	Joback Method
cpg	564.89	J/mol×K	742.74	Joback Method

cpg	577.70	J/mol×K	775.52	Joback Method
cpg	589.75	J/mol×K	808.31	Joback Method
cpg	601.05	J/mol×K	841.09	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=R341872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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