

3-Mercaptohexyl butanoate

Other names:	Butanoic acid, 3-mercaptohexyl ester 3-sulfanylhexyl butanoate
Inchi:	InChI=1S/C10H20O2S/c1-3-5-9(13)7-8-12-10(11)6-4-2/h9,13H,3-8H2,1-2H3
InchiKey:	TZCJKOLXWHXDAF-UHFFFAOYSA-N
Formula:	C10H20O2S
SMILES:	CCCC(=O)OCCC(S)CCC
Mol. weight [g/mol]:	204.33
CAS:	136954-21-7

Physical Properties

Property code	Value	Unit	Source
gf	-173.65	kJ/mol	Joback Method
hf	-461.33	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	53.36	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.818		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
ripol	1821.00		NIST Webbook
ripol	1860.00		NIST Webbook
tb	566.91	K	Joback Method
tc	760.21	K	Joback Method
tf	296.08	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.94	J/mol×K	566.91	Joback Method
cpg	437.78	J/mol×K	599.13	Joback Method
cpg	451.94	J/mol×K	631.34	Joback Method
cpg	465.43	J/mol×K	663.56	Joback Method
cpg	478.26	J/mol×K	695.77	Joback Method

cpg	490.44	J/mol×K	727.99	Joback Method
cpg	501.97	J/mol×K	760.21	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=C136954217&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/45-596-1/3-Mercaptohexyl-butanoate.pdf>

Generated by Cheméo on 2025-12-07 05:55:57.658982232 +0000 UTC m=+4835155.189022886.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.