

4-(Octylthio)butyric acid

Inchi:	InChI=1S/C12H24O2S/c1-2-3-4-5-6-7-10-15-11-8-9-12(13)14/h2-11H2,1H3,(H,13,14)
InchiKey:	GUDSRDGLYIGGNX-UHFFFAOYSA-N
Formula:	C12H24O2S
SMILES:	CCCCCCCCSCCCC(=O)O
Mol. weight [g/mol]:	232.38
CAS:	116346-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-182.46	kJ/mol	Joback Method
hf	-513.95	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	72.55	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.945		Crippen Method
mcvol	203.730	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
tb	688.79	K	Joback Method
tc	868.96	K	Joback Method
tf	370.15	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.69	J/molxK	688.79	Joback Method
cpg	575.34	J/molxK	718.82	Joback Method
cpg	588.32	J/molxK	748.85	Joback Method
cpg	600.64	J/molxK	778.88	Joback Method
cpg	612.31	J/molxK	808.91	Joback Method
cpg	623.36	J/molxK	838.93	Joback Method
cpg	633.81	J/molxK	868.96	Joback Method

Sources

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=C116346237&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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