

4-(Ethylthio)butric acid

Inchi:	InChI=1S/C6H12O2S/c1-2-9-5-3-4-6(7)8/h2-5H2,1H3,(H,7,8)
InchiKey:	DBNZPPFTPCELJG-UHFFFAOYSA-N
Formula:	C6H12O2S
SMILES:	CCSCCCC(=O)O
Mol. weight [g/mol]:	148.22
CAS:	71057-15-3

Physical Properties

Property code	Value	Unit	Source
gf	-232.98	kJ/mol	Joback Method
hf	-390.11	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	59.19	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.604		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	551.51	K	Joback Method
tc	740.73	K	Joback Method
tf	302.53	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.59	J/molxK	551.51	Joback Method
cpg	277.91	J/molxK	583.05	Joback Method
cpg	286.80	J/molxK	614.58	Joback Method
cpg	295.26	J/molxK	646.12	Joback Method
cpg	303.31	J/molxK	677.65	Joback Method
cpg	310.95	J/molxK	709.19	Joback Method
cpg	318.18	J/molxK	740.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71057153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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