

BUTANOIC ACID, 4-(METHYLTHIO)-

Other names:	4-methylthiobutanoic acid
Inchi:	InChI=1S/C5H10O2S/c1-8-4-2-3-5(6)7/h2-4H2,1H3,(H,6,7)
InchiKey:	VDSUAILXEZKWIZ-UHFFFAOYSA-N
Formula:	C5H10O2S
SMILES:	CSCCCC(=O)O
Mol. weight [g/mol]:	134.20

Physical Properties

Property code	Value	Unit	Source
af	0.6547		Cheméo Relay (1.0)
gf	-241.40	kJ/mol	Joback Method
hf	-460.15	kJ/mol	Cheméo Relay (1.0)
hfus	18.52	kJ/mol	Joback Method
hvap	80.69	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	0.14		Cheméo Relay (1.0)
logp	1.214		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
tb	528.31	K	Cheméo Relay (1.0)
tc	729.13	K	Cheméo Relay (1.0)
tf	312.01	K	Cheméo Relay (1.0)
vc	0.357	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.69	J/mol×K	528.63	Joback Method
cpg	233.96	J/mol×K	560.55	Joback Method
cpg	241.86	J/mol×K	592.48	Joback Method
cpg	249.38	J/mol×K	624.40	Joback Method
cpg	256.54	J/mol×K	656.32	Joback Method

cpg	263.34	J/mol×K	688.25	Joback Method
cpg	269.77	J/mol×K	720.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32391972&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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