Butanethioic acid, S-methyl ester

Other names:	Butyric acid, thio-, S-methyl ester
	Methane n-thiolbutyrate
	S-Methyl thiobutyrate
	Methyl thiobutanoate
	s-Methyl thiobutanoate
	Methylthiobutyrate
	S-methyl butanethioate
Inchi:	InChI=1S/C5H10OS/c1-3-4-5(6)7-2/h3-4H2,1-2H3
InchiKey:	GRLJIIJNZJVMGP-UHFFFAOYSA-N
Formula:	C5H10OS
SMILES:	CCCC(=O)SC
Mol. weight [g/mol]:	118.20
CAS:	2432-51-1

Physical Properties

Property code	Value	Unit	Source
gf	-104.58	kJ/mol	Joback Method
hf	-217.24	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	40.29	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.676		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	867.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	867.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1198.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1198.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1195.00		NIST Webbook

tb	436.45	K	Joback Method
tc	639.57	K	Joback Method
tf	230.44	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.53	J/mol×K	436.45	Joback Method
cpg	194.04	J/mol×K	470.30	Joback Method
cpg	203.15	J/mol×K	504.16	Joback Method
cpg	211.86	J/mol×K	538.01	Joback Method
cpg	220.19	J/mol×K	571.86	Joback Method
cpg	228.12	J/mol×K	605.72	Joback Method
cpg	235.68	J/mol×K	639.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.70	K	101.00	NIST Webbook

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=C2432511&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume