(1-methylbutyl) methyl sulfide

Other names: Methyl (1-methylbutyl) sulfide
Inchi: InChI=1S/C6H14S/c1-4-5-6(2)7-3/h6H,4-5H2,1-3H3
InchiKey: WGBHWWSSUGCSCP-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CCCC(C)SC
Mol. weight [g/mol]: 118.24

Physical Properties

Property code	Value	Unit	Source
gf	30.32	kJ/mol	Joback Method
hf	-130.58	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Joback Method
hvap	35.38	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.538		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	868.00		NIST Webbook
tb	405.02	K	Joback Method
tc	598.38	K	Joback Method
tf	176.78	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.46	J/mol×K	405.02	Joback Method
cpg	218.30	J/mol×K	437.25	Joback Method
cpg	229.68	J/mol×K	469.47	Joback Method
cpg	240.61	J/mol×K	501.70	Joback Method
cpg	251.08	J/mol×K	533.93	Joback Method
cpg	261.10	J/mol×K	566.16	Joback Method
cpg	270.69	J/mol×K	598.38	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R130360&Units=SI

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