Butane, 2,3,3-trimethyl-1,2-bis-(methylthio)

Inchi: InChI=1S/C9H20S2/c1-8(2,3)9(4,11-6)7-10-5/h7H2,1-6H3
InchiKey: ILJWLMSOGHPDFW-UHFFFAOYSA-N
Formula: C9H20S2
SMILES: CSCC(C)(SC)C(C)(C)C
Mol. weight [g/mol]: 192.38

Physical Properties

Property code	Value	Unit	Source
gf	96.82	kJ/mol	Joback Method
hf	-162.85	kJ/mol	Joback Method
hfus	12.50	kJ/mol	Joback Method
hvap	46.67	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.517		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1416.00		NIST Webbook
tb	536.42	K	Joback Method
tc	766.34	K	Joback Method
tf	264.83	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.36	J/mol×K	536.42	Joback Method
cpg	410.99	J/mol×K	574.74	Joback Method
cpg	427.42	J/mol×K	613.06	Joback Method
cpg	442.70	J/mol×K	651.38	Joback Method
cpg	456.90	J/mol×K	689.70	Joback Method
cpg	470.08	J/mol×K	728.02	Joback Method
cpg	482.31	J/mol×K	766.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121727&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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