butyl methyl trisulfide

Inchi: InChI=1S/C5H12S3/c1-3-4-5-7-8-6-2/h3-5H2,1-2H3
InchiKey: UERQNAZBAUOZKO-UHFFFAOYSA-N
Formula: C5H12S3
SMILES: CCCCSSSC
Mol. weight [g/mol]: 168.34

Physical Properties

Property code	Value	Unit	Source
gf	90.58	kJ/mol	Joback Method
hf	-20.92	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	47.17	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.446		Crippen Method
mcvol	130.360	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
rinpol	1241.00		NIST Webbook
rinpol	1241.00		NIST Webbook
tb	520.14	K	Joback Method
tc	758.40	K	Joback Method
tf	249.31	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.08	J/mol×K	520.14	Joback Method
cpg	269.75	J/mol×K	559.85	Joback Method
cpg	280.84	J/mol×K	599.56	Joback Method
cpg	291.33	J/mol×K	639.27	Joback Method
cpg	301.21	J/mol×K	678.98	Joback Method
cpg	310.47	J/mol×K	718.69	Joback Method
cpg	319.09	J/mol×K	758.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R63245&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume