

CH3SBrCH2

Inchi:	InChI=1S/C2H5BrS/c1-4-2-3/h2H2,1H3
InchiKey:	DQKDNVFNQRYIS-UHFFFAOYSA-N
Formula:	C2H5BrS
SMILES:	CSCBr
Mol. weight [g/mol]:	141.03
CAS:	24276-77-5

Physical Properties

Property code	Value	Unit	Source
gf	13.40	kJ/mol	Joback Method
hf	-16.41	kJ/mol	Joback Method
hfus	10.35	kJ/mol	Joback Method
hvap	33.30	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.702		Crippen Method
mcvol	72.890	ml/mol	McGowan Method
pc	5704.58	kPa	Joback Method
tb	380.10	K	Joback Method
tc	596.91	K	Joback Method
tf	206.50	K	Joback Method
vc	0.264	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	99.18	J/mol×K	380.10	Joback Method
cpg	104.35	J/mol×K	416.24	Joback Method
cpg	109.27	J/mol×K	452.37	Joback Method
cpg	113.96	J/mol×K	488.51	Joback Method
cpg	118.42	J/mol×K	524.64	Joback Method
cpg	122.65	J/mol×K	560.78	Joback Method
cpg	126.67	J/mol×K	596.91	Joback Method

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=C24276775&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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