

Dibromomethyl radical

Inchi:	InChI=1S/CHBr2/c2-1-3/h1H
InchiKey:	HFPGRVHMFSJMOL-UHFFFAOYSA-N
Formula:	CHBr2
SMILES:	Br[CH]Br
Mol. weight [g/mol]:	172.83
CAS:	14362-13-1

Physical Properties

Property code	Value	Unit	Source
gf	36.12	kJ/mol	Joback Method
hf	39.22	kJ/mol	Joback Method
hfus	7.08	kJ/mol	Joback Method
hvap	30.16	kJ/mol	Joback Method
ie	8.30 ± 0.03	eV	NIST Webbook
ie	8.41 ± 0.03	eV	NIST Webbook
ie	8.13 ± 0.16	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.895		Crippen Method
mcvol	57.800	ml/mol	McGowan Method
pc	7915.30	kPa	Joback Method
tb	353.46	K	Joback Method
tc	566.76	K	Joback Method
tf	222.00	K	Joback Method
vc	0.201	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	56.56	J/molxK	353.46	Joback Method
cpg	59.14	J/molxK	389.01	Joback Method
cpg	61.26	J/molxK	424.56	Joback Method
cpg	62.98	J/molxK	460.11	Joback Method
cpg	64.35	J/molxK	495.66	Joback Method
cpg	65.41	J/molxK	531.21	Joback Method

cpg	66.22	J/mol×K	566.76	Joback Method
dvisc	0.0016191	Paxs	222.00	Joback Method
dvisc	0.0012920	Paxs	243.91	Joback Method
dvisc	0.0010700	Paxs	265.82	Joback Method
dvisc	0.0009120	Paxs	287.73	Joback Method
dvisc	0.0007951	Paxs	309.64	Joback Method
dvisc	0.0007058	Paxs	331.55	Joback Method
dvisc	0.0006359	Paxs	353.46	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=C14362131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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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