

tribromonitromethane

Inchi:	InChI=1S/CBr3NO2/c2-1(3,4)5(6)7
InchiKey:	QQZIUHOKWDFXEY-UHFFFAOYSA-N
Formula:	CBr3NO2
SMILES:	O=[N+](O-)C(Br)(Br)Br
Mol. weight [g/mol]:	297.73
CAS:	464-10-8

Physical Properties

Property code	Value	Unit	Source
gf	38.89	kJ/mol	Joback Method
hf	-4.49	kJ/mol	Joback Method
hfus	18.15	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.059		Crippen Method
mcvol	94.870	ml/mol	McGowan Method
pc	8637.25	kPa	Joback Method
tb	569.37	K	Joback Method
tc	858.80	K	Joback Method
tf	426.46	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.74	J/molxK	569.37	Joback Method
cpg	135.48	J/molxK	617.61	Joback Method
cpg	137.60	J/molxK	665.85	Joback Method
cpg	139.22	J/molxK	714.08	Joback Method
cpg	140.49	J/molxK	762.32	Joback Method
cpg	141.52	J/molxK	810.56	Joback Method
cpg	142.45	J/molxK	858.80	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=C464108&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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