

Trichloroacetamide, N,N-dibutyl-

Inchi:	InChI=1S/C10H18Cl3NO/c1-3-5-7-14(8-6-4-2)9(15)10(11,12)13/h3-8H2,1-2H3
InchiKey:	XAPJKGWLPPCTDF-UHFFFAOYSA-N
Formula:	C10H18Cl3NO
SMILES:	CCCCN(CCCC)C(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	274.62

Physical Properties

Property code	Value	Unit	Source
gf	-17.77	kJ/mol	Joback Method
hf	-350.75	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	58.50	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.785		Crippen Method
mvol	200.030	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1636.00		NIST Webbook
tb	603.57	K	Joback Method
tc	799.01	K	Joback Method
tf	377.04	K	Joback Method
vc	0.755	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.59	J/mol×K	603.57	Joback Method
cpg	483.16	J/mol×K	636.14	Joback Method
cpg	495.89	J/mol×K	668.72	Joback Method
cpg	507.83	J/mol×K	701.29	Joback Method
cpg	519.01	J/mol×K	733.86	Joback Method
cpg	529.50	J/mol×K	766.43	Joback Method
cpg	539.33	J/mol×K	799.01	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=U308485&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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