Trichloroacetamide, N,N-dihexyl-

Inchi: InChI=1S/C14H26Cl3NO/c1-3-5-7-9-11-18(12-10-8-6-4-2)13(19)14(15,16)17/h3-12H2,1-
InchiKey: KUPGOOKIYUHFCE-UHFFFAOYSA-N
Formula: C14H26Cl3NO
SMILES: CCCCCCN(CCCCCC)C(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 330.72

Physical Properties

Property code	Value	Unit	Source
gf	15.91	kJ/mol	Joback Method
hf	-433.31	kJ/mol	Joback Method
hfus	41.81	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.346		Crippen Method
mcvol	256.390	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	695.09	K	Joback Method
tc	883.04	K	Joback Method
tf	422.12	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.97	J/mol×K	695.09	Joback Method
cpg	692.34	J/mol×K	726.42	Joback Method
cpg	706.84	J/mol×K	757.74	Joback Method
cpg	720.51	J/mol×K	789.07	Joback Method
cpg	733.40	J/mol×K	820.39	Joback Method
cpg	745.57	J/mol×K	851.72	Joback Method
cpg	757.07	J/mol×K	883.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308487&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