Trichloroacetamide, N,N-diheptyl-

Inchi: InChI=1S/C16H30Cl3NO/c1-3-5-7-9-11-13-20(15(21)16(17,18)19)14-12-10-8-6-4-2/h3-14
InchiKey: BVFXHEMDRLSTLE-UHFFFAOYSA-N
Formula: C16H30Cl3NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 358.77

Physical Properties

Property code	Value	Unit	Source
gf	32.75	kJ/mol	Joback Method
hf	-474.59	kJ/mol	Joback Method
hfus	46.99	kJ/mol	Joback Method
hvap	71.86	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	6.126		Crippen Method
mcvol	284.570	ml/mol	McGowan Method
pc	1289.29	kPa	Joback Method
rinpol	2216.00		NIST Webbook
tb	740.85	K	Joback Method
tc	927.52	K	Joback Method
tf	444.66	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.04	J/mol×K	740.85	Joback Method
cpg	804.11	J/mol×K	771.96	Joback Method
cpg	819.29	J/mol×K	803.07	Joback Method
cpg	833.63	J/mol×K	834.18	Joback Method
cpg	847.18	J/mol×K	865.30	Joback Method
cpg	860.00	J/mol×K	896.41	Joback Method
cpg	872.14	J/mol×K	927.52	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=U308490&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume