Trichloroacetamide, N,N-bis(2-ethylhexyl)-

Inchi: InChI=1S/C18H34Cl3NO/c1-5-9-11-15(7-3)13-22(17(23)18(19,20)21)14-16(8-4)12-10-6-
InchiKey: AQTKUBSOCLDIJW-UHFFFAOYSA-N
Formula: C18H34Cl3NO
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 386.83

Physical Properties

Property code	Value	Unit	Source
gf	44.71	kJ/mol	Joback Method
hf	-526.43	kJ/mol	Joback Method
hfus	45.13	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.618		Crippen Method
mcvol	312.750	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2188.00		NIST Webbook
rinpol	2188.00		NIST Webbook
tb	785.73	K	Joback Method
tc	976.74	K	Joback Method
tf	437.20	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.29	J/mol×K	785.73	Joback Method
cpg	921.37	J/mol×K	817.57	Joback Method
cpg	937.47	J/mol×K	849.40	Joback Method
cpg	952.66	J/mol×K	881.24	Joback Method
cpg	967.01	J/mol×K	913.07	Joback Method
cpg	980.57	J/mol×K	944.91	Joback Method
cpg	993.41	J/mol×K	976.74	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=U308489&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