Dichloroacetamide, N-heptyl-N-octyl-

Inchi: InChI=1S/C17H33Cl2NO/c1-3-5-7-9-11-13-15-20(17(21)16(18)19)14-12-10-8-6-4-2/h16H
InchiKey: SOTPHTCBQMPAOA-UHFFFAOYSA-N
Formula: C17H33Cl2NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)C(Cl)Cl
Mol. weight [g/mol]: 338.36

Physical Properties

Property code	Value	Unit	Source
gf	47.82	kJ/mol	Joback Method
hf	-476.02	kJ/mol	Joback Method
hfus	49.28	kJ/mol	Joback Method
hvap	70.61	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.950		Crippen Method
mcvol	286.420	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	729.09	K	Joback Method
tc	907.64	K	Joback Method
tf	408.59	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.21	J/mol×K	729.09	Joback Method
cpg	829.52	J/mol×K	758.85	Joback Method
cpg	845.96	J/mol×K	788.61	Joback Method
cpg	861.54	J/mol×K	818.37	Joback Method
cpg	876.32	J/mol×K	848.12	Joback Method
cpg	890.32	J/mol×K	877.88	Joback Method
cpg	903.59	J/mol×K	907.64	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308636&Units=SI

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