Dichloroacetamide, N,N-diheptyl-

Inchi: InChI=1S/C16H31Cl2NO/c1-3-5-7-9-11-13-19(16(20)15(17)18)14-12-10-8-6-4-2/h15H,3-
InchiKey: DTFJMKGUYWLTPF-UHFFFAOYSA-N
Formula: C16H31Cl2NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)C(Cl)Cl
Mol. weight [g/mol]: 324.33

Physical Properties

Property code	Value	Unit	Source
gf	39.40	kJ/mol	Joback Method
hf	-455.38	kJ/mol	Joback Method
hfus	46.69	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.560		Crippen Method
mcvol	272.330	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	2086.00		NIST Webbook
tb	706.21	K	Joback Method
tc	884.39	K	Joback Method
tf	397.32	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.03	J/mol×K	706.21	Joback Method
cpg	771.97	J/mol×K	735.91	Joback Method
cpg	788.05	J/mol×K	765.60	Joback Method
cpg	803.31	J/mol×K	795.30	Joback Method
cpg	817.78	J/mol×K	825.00	Joback Method
cpg	831.50	J/mol×K	854.69	Joback Method
cpg	844.50	J/mol×K	884.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308635&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