

Dichloroacetamide, N,N-dioctyl-

Inchi:	InChI=1S/C18H35Cl2NO/c1-3-5-7-9-11-13-15-21(18(22)17(19)20)16-14-12-10-8-6-4-2/h
InchiKey:	AIUSXCDXRWTYKI-UHFFFAOYSA-N
Formula:	C18H35Cl2NO
SMILES:	CCCCCCCCN(CCCCCCCC)C(=O)C(Cl)Cl
Mol. weight [g/mol]:	352.38

Physical Properties

Property code	Value	Unit	Source
gf	56.24	kJ/mol	Joback Method
hf	-496.66	kJ/mol	Joback Method
hfus	51.87	kJ/mol	Joback Method
hvap	72.83	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.340		Crippen Method
mvol	300.510	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2288.00		NIST Webbook
tb	751.97	K	Joback Method
tc	931.44	K	Joback Method
tf	419.86	K	Joback Method
vc	1.159	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.43	J/mol×K	751.97	Joback Method
cpg	888.12	J/mol×K	781.88	Joback Method
cpg	904.90	J/mol×K	811.79	Joback Method
cpg	920.81	J/mol×K	841.71	Joback Method
cpg	935.88	J/mol×K	871.62	Joback Method
cpg	950.17	J/mol×K	901.53	Joback Method
cpg	963.70	J/mol×K	931.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308637&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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

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