2,2-Dichloro-n,n-diethylpropanamide

Inchi: InChI=1S/C7H13Cl2NO/c1-4-10(5-2)6(11)7(3,8)9/h4-5H2,1-3H3
InchiKey: BCTIPWRWOIIMDL-UHFFFAOYSA-N
Formula: C7H13Cl2NO
SMILES: CCN(CC)C(=O)C(C)(Cl)Cl
Mol. weight [g/mol]: 198.09
CAS: 89693-51-6

Physical Properties

Property code	Value	Unit	Source
gf	-31.10	kJ/mol	Joback Method
hf	-273.09	kJ/mol	Joback Method
hfus	19.49	kJ/mol	Joback Method
hvap	47.44	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.049		Crippen Method
mcvol	145.520	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	497.50	K	Joback Method
tc	696.26	K	Joback Method
tf	313.31	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.54	J/mol×K	497.50	Joback Method
cpg	315.90	J/mol×K	530.63	Joback Method
cpg	327.46	J/mol×K	563.75	Joback Method
cpg	338.27	J/mol×K	596.88	Joback Method
cpg	348.38	J/mol×K	630.01	Joback Method
cpg	357.82	J/mol×K	663.13	Joback Method
cpg	366.63	J/mol×K	696.26	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=C89693516&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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