

N,n'-ethylene bis(a,a-dichloropropionamide)

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C8H12Cl4N2O2/c1-7(9,10)5(15)13-3-4-14-6(16)8(2,11)12/h3-4H2,1-2H3,(H,13)

UDKOFNMEFRQHJV-UHFFFAOYSA-N

C8H12Cl4N2O2

CC(Cl)(Cl)C(=O)NCCNC(=O)C(C)(Cl)Cl

310.00

116402-52-9

Physical Properties

Property code	Value	Unit	Source
gf	-104.62	kJ/mol	Joback Method
hf	-407.13	kJ/mol	Joback Method
hfus	31.83	kJ/mol	Joback Method
hvap	74.71	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	1.606		Crippen Method
mcvol	195.640	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
tb	733.78	K	Joback Method
tc	958.33	K	Joback Method
tf	509.62	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.06	J/molxK	733.78	Joback Method
cpg	478.16	J/molxK	771.21	Joback Method
cpg	486.48	J/molxK	808.63	Joback Method
cpg	494.10	J/molxK	846.06	Joback Method
cpg	501.11	J/molxK	883.48	Joback Method
cpg	507.58	J/molxK	920.91	Joback Method
cpg	513.61	J/molxK	958.33	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=C116402529&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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