

Adipamide, n,n'-bis(2-chloroethyl)-

Inchi:	InChI=1S/C10H18Cl2N2O2/c11-5-7-13-9(15)3-1-2-4-10(16)14-8-6-12/h1-8H2,(H,13,15)(
InchiKey:	KHFRDDZLYGUJBJ-UHFFFAOYSA-N
Formula:	C10H18Cl2N2O2
SMILES:	O=C(CCCCC(=O)NCCCI)NCCCI
Mol. weight [g/mol]:	269.17
CAS:	6265-81-2

Physical Properties

Property code	Value	Unit	Source
gf	-69.60	kJ/mol	Joback Method
hf	-399.43	kJ/mol	Joback Method
hfus	43.45	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.257		Crippen Method
mcvol	199.340	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	711.14	K	Joback Method
tc	904.67	K	Joback Method
tf	467.48	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.73	J/molxK	711.14	Joback Method
cpg	532.51	J/molxK	743.40	Joback Method
cpg	543.59	J/molxK	775.65	Joback Method
cpg	554.00	J/molxK	807.91	Joback Method
cpg	563.77	J/molxK	840.16	Joback Method
cpg	572.93	J/molxK	872.42	Joback Method
cpg	581.49	J/molxK	904.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6265812&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
mccvol:	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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