

Propionamide, 2,3-dichloro-N-propyl-

Inchi: InChI=1S/C6H11Cl2NO/c1-2-3-9-6(10)5(8)4-7/h5H,2-4H2,1H3,(H,9,10)
InchiKey: AOSNLIMWLVSNNQ-UHFFFAOYSA-N
Formula: C6H11Cl2NO
SMILES: CCCN=C(O)C(Cl)CCl
Mol. weight [g/mol]: 184.06

Physical Properties

Property code	Value	Unit	Source
hf	-283.73	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	2.199		Crippen Method
mcvol	131.430	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	579.84	K	Joback Method
tc	775.56	K	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=U415222&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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

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