3',4'-Dichloroenanthoanilide

Inchi: InChI=1S/C13H17Cl2NO/c1-2-3-4-5-6-13(17)16-10-7-8-11(14)12(15)9-10/h7-9H,2-6H2,1
InchiKey: PDFPVADETAQXIR-UHFFFAOYSA-N
Formula: C13H17Cl2NO
SMILES: CCCCCCC(=O)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 274.19

Physical Properties

Property code	Value	Unit	Source
gf	88.34	kJ/mol	Joback Method
hf	-188.65	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	70.08	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.902		Crippen Method
mcvol	206.300	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	712.38	K	Joback Method
tc	925.98	K	Joback Method
tf	450.16	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.89	J/mol×K	712.38	Joback Method
cpg	536.19	J/mol×K	747.98	Joback Method
cpg	548.63	J/mol×K	783.58	Joback Method
cpg	560.24	J/mol×K	819.18	Joback Method
cpg	571.06	J/mol×K	854.78	Joback Method
cpg	581.14	J/mol×K	890.38	Joback Method
cpg	590.50	J/mol×K	925.98	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=R149067&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume