Acetamide, 2-chloro-N-(2,6-diethylphenyl)-

Other names:	Chloro-N-(2,6-diethylphenyl)acetamide
	2-Chloro-N-(2,6-diethylphenyl)acetamide
	N-2'-Chloroacetyl-2,6-diethylaniline
	2-Chloro-2',6'-diethylacetanilide
Inchi:	InChI=1S/C12H16ClNO/c1-3-9-6-5-7-10(4-2)12(9)14-11(15)8-13/h5-7H,3-4,8H2,1-2H3,(H
InchiKey:	LBJVHMAYBNQJBK-UHFFFAOYSA-N
Formula:	C12H16ClNO
SMILES:	CCc1cccc(CC)c1NC(=O)CCl
Mol. weight [g/mol]:	225.72
CAS:	6967-29-9

Physical Properties

Property code	Value	Unit	Source
gf	91.85	kJ/mol	Joback Method
hf	-152.27	kJ/mol	Joback Method
hfus	30.99	kJ/mol	Joback Method
hvap	63.47	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.989		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1721.00		NIST Webbook
rinpol	289.93		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	289.93		NIST Webbook
rinpol	1716.00		NIST Webbook
tb	652.07	K	Joback Method
tc	865.67	K	Joback Method
tf	408.97	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	445.95	J/mol×K	652.07	Joback Method
cpg	459.74	J/mol×K	687.67	Joback Method
cpg	472.68	J/mol×K	723.27	Joback Method
cpg	484.81	J/mol×K	758.87	Joback Method
cpg	496.16	J/mol×K	794.47	Joback Method
cpg	506.75	J/mol×K	830.07	Joback Method
cpg	516.63	J/mol×K	865.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6967299&Units=SI
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

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