3',4'-Dichlorobutyroanilide

Inchi: InChI=1S/C10H11Cl2NO/c1-2-3-10(14)13-7-4-5-8(11)9(12)6-7/h4-6H,2-3H2,1H3,(H,13,1
InchiKey: NNIIRGXUFKHOKI-UHFFFAOYSA-N
Formula: C10H11Cl2NO
SMILES: CCCC(=O)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 232.11

Physical Properties

Property code	Value	Unit	Source
gf	63.08	kJ/mol	Joback Method
hf	-126.73	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	63.41	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.732		Crippen Method
mcvol	164.030	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	643.74	K	Joback Method
tc	868.27	K	Joback Method
tf	416.35	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.05	J/mol×K	643.74	Joback Method
cpg	383.53	J/mol×K	681.16	Joback Method
cpg	394.23	J/mol×K	718.58	Joback Method
cpg	404.19	J/mol×K	756.01	Joback Method
cpg	413.43	J/mol×K	793.43	Joback Method
cpg	421.99	J/mol×K	830.85	Joback Method
cpg	429.91	J/mol×K	868.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149032&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
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

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