Isobutylcarbamate, N-(3,4-dichlorobenzyl)

Inchi: InChI=1S/C12H15Cl2NO2/c1-8(2)7-17-12(16)15-6-9-3-4-10(13)11(14)5-9/h3-5,8H,6-7H2
InchiKey: YZOYRCABPVRISG-UHFFFAOYSA-N
Formula: C12H15Cl2NO2
SMILES: CC(C)COC(=O)NCc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 276.16

Physical Properties

Property code	Value	Unit	Source
gf	-27.52	kJ/mol	Joback Method
hf	-305.51	kJ/mol	Joback Method
hfus	32.86	kJ/mol	Joback Method
hvap	69.88	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.876		Crippen Method
mcvol	198.080	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	711.48	K	Joback Method
tc	929.87	K	Joback Method
tf	446.12	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.83	J/mol×K	711.48	Joback Method
cpg	509.61	J/mol×K	747.88	Joback Method
cpg	521.51	J/mol×K	784.28	Joback Method
cpg	532.56	J/mol×K	820.67	Joback Method
cpg	542.79	J/mol×K	857.07	Joback Method
cpg	552.20	J/mol×K	893.47	Joback Method
cpg	560.83	J/mol×K	929.87	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=R392513&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