Isobutylcarbamate, N-(2,4-dichlorobenzyl)

Inchi: InChI=1S/C11H13Cl2NO2/c1-7(2)6-16-11(15)14-10-4-3-8(12)5-9(10)13/h3-5,7H,6H2,1-2
InchiKey: SFAAIBQKZLICIP-UHFFFAOYSA-N
Formula: C11H13Cl2NO2
SMILES: CC(C)COC(=O)Nc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 262.13

Physical Properties

Property code	Value	Unit	Source
gf	-35.94	kJ/mol	Joback Method
hf	-284.87	kJ/mol	Joback Method
hfus	30.27	kJ/mol	Joback Method
hvap	67.65	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.198		Crippen Method
mcvol	183.990	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1957.00		NIST Webbook
tb	688.60	K	Joback Method
tc	910.62	K	Joback Method
tf	434.85	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.75	J/mol×K	688.60	Joback Method
cpg	457.97	J/mol×K	725.60	Joback Method
cpg	469.35	J/mol×K	762.61	Joback Method
cpg	479.91	J/mol×K	799.61	Joback Method
cpg	489.68	J/mol×K	836.61	Joback Method
cpg	498.66	J/mol×K	873.61	Joback Method
cpg	506.89	J/mol×K	910.62	Joback Method

Sources

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=R392484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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