

Carbanilide, 2,2'-ditertiary butyl-

Inchi:	InChI=1S/C21H28N2O/c1-20(2,3)15-11-7-9-13-17(15)22-19(24)23-18-14-10-8-12-16(18)
InchiKey:	SBOKLRVCVSYVIH-UHFFFAOYSA-N
Formula:	C21H28N2O
SMILES:	CC(C)(C)c1ccccc1NC(=O)Nc1ccccc1C(C)(C)C
Mol. weight [g/mol]:	324.46

Physical Properties

Property code	Value	Unit	Source
gf	387.04	kJ/mol	Joback Method
hf	-49.79	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	85.24	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.926		Crippen Method
mcvol	280.760	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
tb	890.95	K	Joback Method
tc	1128.24	K	Joback Method
tf	564.40	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.63	J/molxK	890.95	Joback Method
cpg	899.72	J/molxK	930.50	Joback Method
cpg	914.68	J/molxK	970.05	Joback Method
cpg	928.64	J/molxK	1009.60	Joback Method
cpg	941.76	J/molxK	1049.14	Joback Method
cpg	954.18	J/molxK	1088.69	Joback Method
cpg	966.04	J/molxK	1128.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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