

Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate

Other names:

Carbamic acid, methyl-, 2,6-di-tert-butyl-p-tolyl ester

Azak

Terbutol

Terbucarb

MBPMC

Inchi: InChI=1S/C17H27NO2/c1-11-9-12(16(2,3)4)14(20-15(19)18-8)13(10-11)17(5,6)7/h9-10H

InchiKey: PNRAZZISDRWMV-UHFFFAOYSA-N

Formula: C17H27NO2

SMILES: CNC(=O)Oc1c(C(C)(C)C)cc(C)cc1C(C)(C)C

Mol. weight [g/mol]: 277.40

CAS: 1918-11-2

Physical Properties

Property code	Value	Unit	Source
gf	36.93	kJ/mol	Joback Method
hf	-400.92	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.308		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	749.98	K	Joback Method
tc	964.67	K	Joback Method
tf	474.99	K	Joback Method
vc	0.916	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.88	J/mol×K	749.98	Joback Method
cpg	734.17	J/mol×K	785.76	Joback Method
cpg	750.33	J/mol×K	821.54	Joback Method
cpg	765.41	J/mol×K	857.33	Joback Method
cpg	779.47	J/mol×K	893.11	Joback Method
cpg	792.58	J/mol×K	928.89	Joback Method
cpg	804.81	J/mol×K	964.67	Joback Method

Sources

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=C1918112&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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