

tert-Butyl

4-[[[(1,4-dimethyl-2-phenoxy-pyrrol-3-yl)methylene]amino]oxy]methyl]-

Other names: Benzoic acid, 4-[[[(E)-[(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)methylene]amino]oxy]methyl]-, 1,1-dimethylethyl ester

Inchi: InChI=1S/C16H20N2O3/c1-9(2)16(4)15(20)17-13(18-16)12-8-10(3)6-7-11(12)14(19)21-5

InchiKey: FFCCBBNQPIMUJI-UHFFFAOYSA-N

Formula: C16H20N2O3

SMILES: COC(=O)c1ccc(C)cc1C1=NC(C)(C(C)C)C(=O)N1

Mol. weight [g/mol]: 288.34

CAS: 134098-61-6

Physical Properties

Property code	Value	Unit	Source
gf	73.92	kJ/mol	Joback Method
hf	-316.95	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	80.85	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.073		Crippen Method
mcvol	226.350	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	867.70	K	Joback Method
tc	1119.87	K	Joback Method
tf	671.57	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.74	J/molxK	867.70	Joback Method
cpg	734.50	J/molxK	909.73	Joback Method
cpg	751.29	J/molxK	951.76	Joback Method
cpg	767.22	J/molxK	993.78	Joback Method
cpg	782.38	J/molxK	1035.81	Joback Method

cpg	796.84	J/mol×K	1077.84	Joback Method
cpg	810.71	J/mol×K	1119.87	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=C134098616&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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