

1-Phenyl-1,1-di-o-tolyl-2-propanone

Inchi:	InChI=1S/C23H22O/c1-17-11-7-9-15-21(17)23(19(3)24,20-13-5-4-6-14-20)22-16-10-8-12
InchiKey:	GMOUGOGLADCJGU-UHFFFAOYSA-N
Formula:	C23H22O
SMILES:	CC(=O)C(c1ccccc1)(c1ccccc1C)c1ccccc1C
Mol. weight [g/mol]:	314.42
CAS:	6324-65-8

Physical Properties

Property code	Value	Unit	Source
gf	334.67	kJ/mol	Joback Method
hf	47.27	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.227		Crippen Method
mcvol	265.220	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
tb	866.28	K	Joback Method
tc	1125.71	K	Joback Method
tf	505.62	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.77	J/molxK	866.28	Joback Method
cpg	804.38	J/molxK	909.52	Joback Method
cpg	819.57	J/molxK	952.76	Joback Method
cpg	833.51	J/molxK	995.99	Joback Method
cpg	846.38	J/molxK	1039.23	Joback Method
cpg	858.34	J/molxK	1082.47	Joback Method
cpg	869.57	J/molxK	1125.71	Joback Method
dvisc	0.0006350	Paxs	505.62	Joback Method
dvisc	0.0003409	Paxs	565.73	Joback Method

dvisc	0.0002062	Paxs	625.84	Joback Method
dvisc	0.0001362	Paxs	685.95	Joback Method
dvisc	0.0000962	Paxs	746.06	Joback Method
dvisc	0.0000716	Paxs	806.17	Joback Method
dvisc	0.0000555	Paxs	866.28	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=C6324658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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