

1,3,5-Triphenyl-1,5-pentanedione

Inchi:	InChI=1S/C23H20O2/c24-22(19-12-6-2-7-13-19)16-21(18-10-4-1-5-11-18)17-23(25)20-1
InchiKey:	SQFIJFCIFAVGEG-UHFFFAOYSA-N
Formula:	C23H20O2
SMILES:	O=C(CC(CC(=O)c1ccccc1)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	328.40
CAS:	6263-84-9

Physical Properties

Property code	Value	Unit	Source
gf	219.73	kJ/mol	Joback Method
hf	-38.90	kJ/mol	Joback Method
hfus	37.12	kJ/mol	Joback Method
hvap	86.72	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.316		Crippen Method
mcvol	266.790	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
tb	912.98	K	Joback Method
tc	1167.40	K	Joback Method
tf	513.09	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.04	J/molxK	912.98	Joback Method
cpg	815.32	J/molxK	955.38	Joback Method
cpg	828.28	J/molxK	997.79	Joback Method
cpg	840.06	J/molxK	1040.19	Joback Method
cpg	850.81	J/molxK	1082.59	Joback Method
cpg	860.67	J/molxK	1125.00	Joback Method
cpg	869.79	J/molxK	1167.40	Joback Method
dvisc	0.0008604	Paxs	513.09	Joback Method
dvisc	0.0004290	Paxs	579.74	Joback Method

dvisc	0.0002469	Paxs	646.39	Joback Method
dvisc	0.0001575	Paxs	713.03	Joback Method
dvisc	0.0001085	Paxs	779.68	Joback Method
dvisc	0.0000793	Paxs	846.33	Joback Method
dvisc	0.0000607	Paxs	912.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6263849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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