

1,2,4-Triphenyl-1,4-butanedione

Other names:	1,4-Butanedione, 1,2,4-triphenyl-
Inchi:	InChI=1S/C22H18O2/c23-21(18-12-6-2-7-13-18)16-20(17-10-4-1-5-11-17)22(24)19-14-8
InchiKey:	UDJIUKWJBHQMBG-UHFFFAOYSA-N
Formula:	C22H18O2
SMILES:	O=C(CC(C(=O)c1ccccc1)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	314.38
CAS:	4441-01-4

Physical Properties

Property code	Value	Unit	Source
gf	211.31	kJ/mol	Joback Method
hf	-18.26	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	84.50	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	4.926		Crippen Method
mcvol	252.700	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
tb	890.10	K	Joback Method
tc	1149.02	K	Joback Method
tf	501.82	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.79	J/molxK	890.10	Joback Method
cpg	802.61	J/molxK	1105.87	Joback Method
cpg	792.99	J/molxK	1062.72	Joback Method
cpg	782.45	J/molxK	1019.56	Joback Method
cpg	770.84	J/molxK	976.41	Joback Method
cpg	758.00	J/molxK	933.25	Joback Method
cpg	811.44	J/molxK	1149.02	Joback Method
dvisc	0.0000696	Paxs	890.10	Joback Method

dvisc	0.0000907	Paxs	825.39	Joback Method
dvisc	0.0001238	Paxs	760.67	Joback Method
dvisc	0.0001789	Paxs	695.96	Joback Method
dvisc	0.0002787	Paxs	631.25	Joback Method
dvisc	0.0004808	Paxs	566.53	Joback Method
dvisc	0.0009544	Paxs	501.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4441014&Units=SI

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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