1,3,5-Triphenyl-1,5-pentadione

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]: 328.41

Physical Properties

Property code	Value	Unit	Source
af	0.6858		Cheméo Relay (1.0)
gf	219.73	kJ/mol	Joback Method
hf	-24.16	kJ/mol	Cheméo Relay (1.0)
hfus	37.12	kJ/mol	Joback Method
hvap	123.18	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-5.40		Cheméo Relay (1.0)
logp	5.316		Crippen Method
mcvol	266.790	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
tb	672.76	K	Cheméo Relay (1.0)
tc	1004.60	K	Cheméo Relay (1.0)
tf	393.55	K	Cheméo Relay (1.0)
vc	0.944	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.04	J/mol×K	912.98	Joback Method
cpg	815.32	J/mol×K	955.38	Joback Method
cpg	828.28	J/mol×K	997.79	Joback Method
cpg	840.06	J/mol×K	1040.19	Joback Method
cpg	850.81	J/mol×K	1082.59	Joback Method
cpg	860.67	J/mol×K	1125.00	Joback Method
cpg	869.79	J/mol×K	1167.40	Joback Method
dvisc	0.0008604	Pa×s	513.09	Joback Method

dvisc	0.0004290	Pa×s	579.74	Joback Method
dvisc	0.0002469	Pa×s	646.39	Joback Method
dvisc	0.0001575	Pa×s	713.03	Joback Method
dvisc	0.0001085	Pa×s	779.68	Joback Method
dvisc	0.0000793	Pa×s	846.33	Joback Method
dvisc	0.0000607	Pa×s	912.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6263849&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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