

3,3,3-Triphenylpropionic acid

Other names:	Tritylacetic acid 2-Triphenylmethyl acetic acid Benzenepropanoic acid, «beta», «beta»-diphenyl-
Inchi:	InChI=1S/C21H18O2/c22-20(23)16-21(17-10-4-1-5-11-17,18-12-6-2-7-13-18)19-14-8-3-9
InchiKey:	XMSJLUKCGWQAHO-UHFFFAOYSA-N
Formula:	C21H18O2
SMILES:	O=C(O)CC(c1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	302.37
CAS:	900-91-4

Physical Properties

Property code	Value	Unit	Source
gf	200.27	kJ/mol	Joback Method
hf	-40.74	kJ/mol	Joback Method
hfus	30.54	kJ/mol	Joback Method
hvap	91.30	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.496		Crippen Method
mcvol	242.910	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	902.74	K	Joback Method
tc	1150.28	K	Joback Method
tf	518.86	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.89	J/molxK	902.74	Joback Method
cpg	783.07	J/molxK	1109.02	Joback Method
cpg	773.41	J/molxK	1067.77	Joback Method
cpg	763.22	J/molxK	1026.51	Joback Method
cpg	752.35	J/molxK	985.25	Joback Method
cpg	740.62	J/molxK	944.00	Joback Method

cpg	792.38	J/mol×K	1150.28	Joback Method
dvisc	0.0000102	Paxs	902.74	Joback Method
dvisc	0.0000150	Paxs	838.76	Joback Method
dvisc	0.0000236	Paxs	774.78	Joback Method
dvisc	0.0000403	Paxs	710.80	Joback Method
dvisc	0.0000763	Paxs	646.82	Joback Method
dvisc	0.0001665	Paxs	582.84	Joback Method
dvisc	0.0004401	Paxs	518.86	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=C900914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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