

1,3,5-Tribenzoylbenzene

Other names:	Methanone, 1,3,5-benzenetriyltris[phenyl-
Inchi:	InChI=1S/C27H18O3/c28-25(19-10-4-1-5-11-19)22-16-23(26(29)20-12-6-2-7-13-20)18-2
InchiKey:	FDSRSUAVHPFWGT-UHFFFAOYSA-N
Formula:	C27H18O3
SMILES:	O=C(c1ccccc1)c1cc(C(=O)c2ccccc2)cc(C(=O)c2ccccc2)c1
Mol. weight [g/mol]:	390.43
CAS:	25871-69-6

Physical Properties

Property code	Value	Unit	Source
gf	220.08	kJ/mol	Joback Method
hf	-15.17	kJ/mol	Joback Method
hfus	45.87	kJ/mol	Joback Method
hvap	106.36	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	5.380		Crippen Method
mcvol	300.960	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
tb	1095.45	K	Joback Method
tc	1371.79	K	Joback Method
tf	674.56	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.34	J/molxK	1095.45	Joback Method
cpg	967.63	J/molxK	1325.73	Joback Method
cpg	960.16	J/molxK	1279.68	Joback Method
cpg	952.29	J/molxK	1233.62	Joback Method
cpg	943.82	J/molxK	1187.56	Joback Method
cpg	934.58	J/molxK	1141.51	Joback Method
cpg	974.91	J/molxK	1371.79	Joback Method
dvisc	0.0000394	Paxs	1095.45	Joback Method

dvisc	0.0000494	Paxs	1025.30	Joback Method
dvisc	0.0000640	Paxs	955.15	Joback Method
dvisc	0.0000865	Paxs	885.01	Joback Method
dvisc	0.0001230	Paxs	814.86	Joback Method
dvisc	0.0001870	Paxs	744.71	Joback Method
dvisc	0.0003101	Paxs	674.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	533.20	K	0.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25871696&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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