Butanedinitrile, tetraphenyl-

Other names:	1,2-Dicyano-tetraphenyl-ethane
Inchi:	InChI=1S/C28H20N2/c29-21-27(23-13-5-1-6-14-23,24-15-7-2-8-16-24)28(22-30,25-17-9-
InchiKey:	HHDUQHBAZZHUDC-UHFFFAOYSA-N
Formula:	C28H20N2
SMILES:	N#CC(c1ccccc1)(c1ccccc1)C(C#N)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	384.47
CAS:	3122-21-2

Physical Properties

Property code	Value	Unit	Source
gf	906.56	kJ/mol	Joback Method
hf	637.13	kJ/mol	Joback Method
hfus	32.62	kJ/mol	Joback Method
hvap	105.39	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.006		Crippen Method
mcvol	313.100	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
tb	1144.46	K	Joback Method
tc	1440.13	K	Joback Method
tf	645.82	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.05	J/mol×K	1144.46	Joback Method
cpg	1003.35	J/mol×K	1193.74	Joback Method
cpg	1018.04	J/mol×K	1243.02	Joback Method
cpg	1033.54	J/mol×K	1292.29	Joback Method
cpg	1050.24	J/mol×K	1341.57	Joback Method
cpg	1068.53	J/mol×K	1390.85	Joback Method
cpg	1088.81	J/mol×K	1440.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3122212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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