

1,2,3,4-tetraethylbenzene

Inchi:	InChI=1S/C14H22/c1-5-11-9-10-12(6-2)14(8-4)13(11)7-3/h9-10H,5-8H2,1-4H3
InchiKey:	FEWANSQOXSIFOK-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	CCc1ccc(CC)c(CC)c1CC
Mol. weight [g/mol]:	190.33

Physical Properties

Property code	Value	Unit	Source
af	0.5620		KDB
gf	150.52	kJ/mol	Joback Method
hf	-130.17	kJ/mol	Joback Method
hfus	24.89	kJ/mol	Joback Method
hvap	51.02	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.936		Crippen Method
mvol	184.360	ml/mol	McGowan Method
pc	1930.00	kPa	KDB
tb	524.20	K	KDB
tc	708.20	K	KDB
tf	285.00	K	KDB
vc	0.712	m ³ /kmol	KDB
zc	0.2332060		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.27	J/mol×K	561.34	Joback Method
cpg	521.83	J/mol×K	725.58	Joback Method
cpg	507.66	J/mol×K	692.73	Joback Method
cpg	492.74	J/mol×K	659.89	Joback Method
cpg	477.05	J/mol×K	627.04	Joback Method
cpg	460.57	J/mol×K	594.19	Joback Method
cpg	535.27	J/mol×K	758.43	Joback Method
dvisc	0.0001675	Paxs	561.34	Joback Method

dvisc	0.0002078	Paxs	519.70	Joback Method
dvisc	0.0002676	Paxs	478.07	Joback Method
dvisc	0.0003615	Paxs	436.43	Joback Method
dvisc	0.0005205	Paxs	394.79	Joback Method
dvisc	0.0008167	Paxs	353.16	Joback Method
dvisc	0.0014453	Paxs	311.52	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.chemie.org/files/research/kdb/mol/mol708.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.chemie.com/doc/models/crippen_log10ws

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
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
zc:	Critical Compressibility

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