1,4-Bis(2-pentyl)benzene

Inchi: InChI=1S/C16H26/c1-5-7-13(3)15-9-11-16(12-10-15)14(4)8-6-2/h9-14H,5-8H2,1-4H3
InchiKey: PYLNSOZDIJWEEM-UHFFFAOYSA-N
Formula: C16H26
SMILES: CCCC(C)c1ccc(C(C)CCC)cc1
Mol. weight [g/mol]: 218.38
CAS: 1020-14-0

Physical Properties

Property code	Value	Unit	Source
gf	181.74	kJ/mol	Joback Method
hf	-159.07	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.494		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
tb	538.15 ± 2.50	K	NIST Webbook
tc	793.83	K	Joback Method
tf	279.02	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.90	J/mol×K	596.26	Joback Method
cpg	565.57	J/mol×K	629.19	Joback Method
cpg	584.20	J/mol×K	662.12	Joback Method
cpg	601.82	J/mol×K	695.05	Joback Method
cpg	618.49	J/mol×K	727.97	Joback Method
cpg	634.22	J/mol×K	760.90	Joback Method
cpg	649.07	J/mol×K	793.83	Joback Method
dvisc	0.0046147	Pa×s	279.02	Joback Method
dvisc	0.0015822	Pa×s	331.89	Joback Method

dvisc	0.0007280	Pa×s	384.77	Joback Method
dvisc	0.0004041	Pa×s	437.64	Joback Method
dvisc	0.0002546	Pa×s	490.51	Joback Method
dvisc	0.0001756	Pa×s	543.39	Joback Method
dvisc	0.0001293	Pa×s	596.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1020140&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

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