

1,2-Bis(4-butrylphenyl)ethane

Inchi:	InChI=1S/C22H26O2/c1-3-5-21(23)19-13-9-17(10-14-19)7-8-18-11-15-20(16-12-18)22(2
InchiKey:	LFSJWEZPAHCXES-UHFFFAOYSA-N
Formula:	C22H26O2
SMILES:	CCCC(=O)c1ccc(CCc2ccc(C(=O)CCC)cc2)cc1
Mol. weight [g/mol]:	322.44
CAS:	17302-71-5

Physical Properties

Property code	Value	Unit	Source
gf	82.08	kJ/mol	Joback Method
hf	-272.45	kJ/mol	Joback Method
hfus	43.24	kJ/mol	Joback Method
hvap	83.93	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	5.437		Crippen Method
mcvol	276.460	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
tb	873.82	K	Joback Method
tc	1096.92	K	Joback Method
tf	515.44	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.80	J/mol×K	873.82	Joback Method
cpg	907.96	J/mol×K	1059.73	Joback Method
cpg	896.59	J/mol×K	1022.55	Joback Method
cpg	884.27	J/mol×K	985.37	Joback Method
cpg	870.91	J/mol×K	948.19	Joback Method
cpg	856.44	J/mol×K	911.00	Joback Method
cpg	918.45	J/mol×K	1096.92	Joback Method
dvisc	0.0000766	Pa×s	873.82	Joback Method
dvisc	0.0000972	Pa×s	814.09	Joback Method

dvisc	0.0001281	Pa×s	754.36	Joback Method
dvisc	0.0001770	Pa×s	694.63	Joback Method
dvisc	0.0002599	Pa×s	634.90	Joback Method
dvisc	0.0004136	Pa×s	575.17	Joback Method
dvisc	0.0007327	Pa×s	515.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17302715&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
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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