

4-Bromo-2,6-di-sec-butyl phenol

Inchi:	InChI=1S/C14H21BrO/c1-5-9(3)12-7-11(15)8-13(14(12)16)10(4)6-2/h7-10,16H,5-6H2,1-4
InchiKey:	JUVSQNQHCSDIF-UHFFFAOYSA-N
Formula:	C14H21BrO
SMILES:	CCC(C)c1cc(Br)cc(C(C)CC)c1O
Mol. weight [g/mol]:	285.22
CAS:	64080-14-4

Physical Properties

Property code	Value	Unit	Source
gf	14.97	kJ/mol	Joback Method
hf	-280.24	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.182		Crippen Method
mcvol	207.730	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
tb	702.26	K	Joback Method
tc	927.72	K	Joback Method
tf	440.52	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.24	J/molxK	702.26	Joback Method
cpg	562.53	J/molxK	739.84	Joback Method
cpg	576.95	J/molxK	777.41	Joback Method
cpg	590.58	J/molxK	814.99	Joback Method
cpg	603.54	J/molxK	852.56	Joback Method
cpg	615.90	J/molxK	890.14	Joback Method
cpg	627.77	J/molxK	927.72	Joback Method
dvisc	0.0005563	Paxs	440.52	Joback Method
dvisc	0.0002247	Paxs	484.14	Joback Method

dvisc	0.0001054	Paxs	527.77	Joback Method
dvisc	0.0000555	Paxs	571.39	Joback Method
dvisc	0.0000320	Paxs	615.01	Joback Method
dvisc	0.0000199	Paxs	658.64	Joback Method
dvisc	0.0000131	Paxs	702.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64080144&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
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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