

4,4'-(6-T-butyl-m-cresol)isobutyridene

Inchi:	InChI=1S/C26H38O2/c1-15(2)24(18-13-20(25(5,6)7)22(27)11-16(18)3)19-14-21(26(8,9)1
InchiKey:	CSOQDRZGMGKOGN-UHFFFAOYSA-N
Formula:	C26H38O2
SMILES:	Cc1cc(O)c(C(C)(C)C)cc1C(c1cc(C(C)(C)C)c(O)cc1C)C(C)C
Mol. weight [g/mol]:	382.58
CAS:	1843-24-9

Physical Properties

Property code	Value	Unit	Source
gf	45.90	kJ/mol	Joback Method
hf	-535.47	kJ/mol	Joback Method
hfus	39.31	kJ/mol	Joback Method
hvap	103.33	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	7.098		Crippen Method
mcvol	341.420	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
tb	1021.46	K	Joback Method
tc	1266.09	K	Joback Method
tf	683.98	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.71	J/mol×K	1021.46	Joback Method
cpg	1193.29	J/mol×K	1062.23	Joback Method
cpg	1215.03	J/mol×K	1103.00	Joback Method
cpg	1237.22	J/mol×K	1143.77	Joback Method
cpg	1260.11	J/mol×K	1184.54	Joback Method
cpg	1283.97	J/mol×K	1225.31	Joback Method
cpg	1309.08	J/mol×K	1266.09	Joback Method
dvisc	0.0000012	Pa×s	683.98	Joback Method
dvisc	0.0000005	Pa×s	740.23	Joback Method

dvisc	0.0000002	Pa×s	796.47	Joback Method
dvisc	0.0000001	Pa×s	852.72	Joback Method
dvisc	6.3459749e-08	Pa×s	908.97	Joback Method
dvisc	3.7507178e-08	Pa×s	965.21	Joback Method
dvisc	2.3489964e-08	Pa×s	1021.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1843249&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

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