t-Butyldiphenylmethanol

Other names: tert-Butyldiphenylmethanol
Inchi: InChI=1S/C17H20O/c1-16(2,3)17(18,14-10-6-4-7-11-14)15-12-8-5-9-13-15/h4-13,18H,1-
InchiKey: YOVSPPKJDDWJML-UHFFFAOYSA-N
Formula: C17H20O
SMILES: CC(C)(C)C(O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 240.34
CAS: 1657-60-9

Physical Properties

Property code	Value	Unit	Source
gf	185.94	kJ/mol	Joback Method
hf	-90.88	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	72.08	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.969		Crippen Method
mcvol	208.740	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
tb	727.44	K	Joback Method
tc	959.44	K	Joback Method
tf	399.85	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.17	J/mol×K	727.44	Joback Method
cpg	607.08	J/mol×K	766.11	Joback Method
cpg	621.70	J/mol×K	804.77	Joback Method
cpg	635.18	J/mol×K	843.44	Joback Method
cpg	647.66	J/mol×K	882.11	Joback Method
cpg	659.27	J/mol×K	920.77	Joback Method
cpg	670.15	J/mol×K	959.44	Joback Method
dvisc	0.0023220	Pa×s	399.85	Joback Method

dvisc	0.0006616	Pa×s	454.45	Joback Method
dvisc	0.0002468	Pa×s	509.05	Joback Method
dvisc	0.0001114	Pa×s	563.64	Joback Method
dvisc	0.0000579	Pa×s	618.24	Joback Method
dvisc	0.0000335	Pa×s	672.84	Joback Method
dvisc	0.0000210	Pa×s	727.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.00	K	0.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1657609&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume