trans-3-t-Butylcyclobutanol

Inchi: InChI=1S/C8H16O/c1-8(2,3)6-4-7(9)5-6/h6-7,9H,4-5H2,1-3H3/t6-,7-
InchiKey: QTUJAHPEPCHIKC-LJGSYFOKSA-N
Formula: C8H16O
SMILES: CC(C)(C)C1CC(O)C1
Mol. weight [g/mol]: 128.21
CAS: 20476-25-9

Physical Properties

Property code	Value	Unit	Source
gf	-76.56	kJ/mol	Joback Method
hf	-323.13	kJ/mol	Joback Method
hfus	10.26	kJ/mol	Joback Method
hvap	48.56	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.803		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	477.73	K	Joback Method
tc	665.75	K	Joback Method
tf	253.34	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.61	J/mol×K	477.73	Joback Method
cpg	344.04	J/mol×K	634.41	Joback Method
cpg	332.43	J/mol×K	603.08	Joback Method
cpg	320.13	J/mol×K	571.74	Joback Method
cpg	307.08	J/mol×K	540.40	Joback Method
cpg	293.25	J/mol×K	509.07	Joback Method
cpg	354.98	J/mol×K	665.75	Joback Method
dvisc	0.0002827	Pa×s	477.73	Joback Method
dvisc	0.0004388	Pa×s	440.33	Joback Method

dvisc	0.0007391	Pa×s	402.93	Joback Method
dvisc	0.0013851	Pa×s	365.53	Joback Method
dvisc	0.0029953	Pa×s	328.14	Joback Method
dvisc	0.0078992	Pa×s	290.74	Joback Method
dvisc	0.0277371	Pa×s	253.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20476259&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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