1,2-Benzenediol, 3,5-bis(1,1-dimethylethyl)-

Other names: 1,2-Benzenediol, 3,5-di(1,1-dimethylethyl)-
3,5-di-tert-Butylcatechol
3,5-di-t-Butylcatechol
Pyrocatechol, 3,5-di-tert-butyl-
3,5-Di-tert-butylpyrocatechol
4,6-Di-tert-butylpyrocatechol
3,5-Di-tert-butyl-1,2-benzenediol
3,5-Bis(1,1-dimethylethyl)catechol
NSC 59767

Inchi: InChI=1S/C14H22O2/c1-13(2,3)9-7-10(14(4,5)6)12(16)11(15)8-9/h7-8,15-16H,1-6H3

InchiKey: PJZLSMMERMMQBJ-UHFFFAOYSA-N

Formula: C14H22O2

SMILES: CC(C)(C)c1cc(O)c(O)c(C(C)(C)C)c1

Mol. weight [g/mol]: 222.32

CAS: 1020-31-1

Physical Properties

Property code	Value	Unit	Source
chs	-8082.70 ± 1.80	kJ/mol	NIST Webbook
gf	-133.78	kJ/mol	Joback Method
hf	-470.50 ± 2.70	kJ/mol	NIST Webbook
hfs	-570.60 ± 2.60	kJ/mol	NIST Webbook
hfus	22.41	kJ/mol	Joback Method
hsub	100.10 ± 0.60	kJ/mol	NIST Webbook
hsub	104.70 ± 0.50	kJ/mol	NIST Webbook
hsub	100.10	kJ/mol	NIST Webbook
hsub	100.10 ± 0.60	kJ/mol	NIST Webbook
hvap	73.13	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.693		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1683.00		NIST Webbook
tb	706.16	K	Joback Method
tc	944.46	K	Joback Method
tf	514.76	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.41	J/mol×K	904.74	Joback Method
cpg	649.38	J/mol×K	944.46	Joback Method
cpg	566.27	J/mol×K	706.16	Joback Method
cpg	581.71	J/mol×K	745.88	Joback Method
cpg	596.24	J/mol×K	785.59	Joback Method
cpg	610.05	J/mol×K	825.31	Joback Method
cpg	623.37	J/mol×K	865.02	Joback Method
dvisc	0.0000010	Pa×s	706.16	Joback Method
dvisc	0.0000016	Pa×s	674.26	Joback Method
dvisc	0.0000430	Pa×s	514.76	Joback Method
dvisc	0.0000192	Pa×s	546.66	Joback Method
dvisc	0.0000094	Pa×s	578.56	Joback Method
dvisc	0.0000049	Pa×s	610.46	Joback Method
dvisc	0.0000028	Pa×s	642.36	Joback Method
hfust	24.10	kJ/mol	372.80	NIST Webbook
hsubt	103.70 ± 0.50	kJ/mol	330.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1020311&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume