Benzene, 1,3-dimethyl-2,4,6-tris-(1-methylethyl)

Inchi: InChI=1S/C17H28/c1-10(2)15-9-16(11(3)4)14(8)17(12(5)6)13(15)7/h9-12H,1-8H3
InchiKey: PROKPBMWEXYEFG-UHFFFAOYSA-N
Formula: C17H28
SMILES: Cc1c(C(C)C)cc(C(C)C)c(C)c1C(C)C
Mol. weight [g/mol]: 232.40

Physical Properties

Property code	Value	Unit	Source
gf	158.83	kJ/mol	Joback Method
hf	-219.40	kJ/mol	Joback Method
hfus	21.70	kJ/mol	Joback Method
hvap	57.20	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.674		Crippen Method
mcvol	226.630	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
ripol	1794.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	633.64	K	Joback Method
tc	835.03	K	Joback Method
tf	312.85	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.85	J/mol×K	633.64	Joback Method
cpg	620.66	J/mol×K	667.21	Joback Method
cpg	639.47	J/mol×K	700.77	Joback Method
cpg	657.30	J/mol×K	734.34	Joback Method
cpg	674.20	J/mol×K	767.90	Joback Method
cpg	690.17	J/mol×K	801.47	Joback Method

cpg	705.26	J/mol×K	835.03	Joback Method
dvisc	0.0021048	Pa×s	312.85	Joback Method
dvisc	0.0008867	Pa×s	366.31	Joback Method
dvisc	0.0004656	Pa×s	419.78	Joback Method
dvisc	0.0002827	Pa×s	473.25	Joback Method
dvisc	0.0001900	Pa×s	526.71	Joback Method
dvisc	0.0001374	Pa×s	580.17	Joback Method
dvisc	0.0001049	Pa×s	633.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R555972&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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