Benzene, 1-methyl-3,5-bis(1-methylethyl)-

Other names: 1,3-Di-isopropyl-5-methylbenzene
Toluene, 3,5-diisopropyl-
Inchi: InChI=1S/C13H20/c1-9(2)12-6-11(5)7-13(8-12)10(3)4/h6-10H,1-5H3
InchiKey: SOALUUXENHDLMW-UHFFFAOYSA-N
Formula: C13H20
SMILES: Cc1cc(C(C)C)cc(C(C)C)c1
Mol. weight [g/mol]: 176.30
CAS: 3055-14-9

Physical Properties

Property code	Value	Unit	Source
gf	146.85	kJ/mol	Joback Method
hf	-108.62	kJ/mol	Joback Method
hfus	15.64	kJ/mol	Joback Method
hvap	47.36	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.242		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
tb	532.60	K	Joback Method
tc	740.08	K	Joback Method
tf	212.00 ± 1.00	K	NIST Webbook
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.49	J/mol×K	532.60	Joback Method
cpg	412.29	J/mol×K	567.18	Joback Method
cpg	429.16	J/mol×K	601.76	Joback Method
cpg	445.14	J/mol×K	636.34	Joback Method
cpg	460.25	J/mol×K	670.92	Joback Method

cpg	474.53	J/mol×K	705.50	Joback Method
cpg	488.00	J/mol×K	740.08	Joback Method
dvisc	0.0035478	Pa×s	257.73	Joback Method
dvisc	0.0014389	Pa×s	303.54	Joback Method
dvisc	0.0007394	Pa×s	349.35	Joback Method
dvisc	0.0004434	Pa×s	395.17	Joback Method
dvisc	0.0002957	Pa×s	440.98	Joback Method
dvisc	0.0002128	Pa×s	486.79	Joback Method
dvisc	0.0001621	Pa×s	532.60	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=C3055149&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume