

1,3,5-Triisopropyl-2-methylbenzene

Inchi:	InChI=1S/C16H26/c1-10(2)14-8-15(11(3)4)13(7)16(9-14)12(5)6/h8-12H,1-7H3
InchiKey:	CHVOYGXBBWPDEU-UHFFFAOYSA-N
Formula:	C16H26
SMILES:	Cc1c(C(C)C)cc(C(C)C)cc1C(C)C
Mol. weight [g/mol]:	218.38
CAS:	6319-85-3

Physical Properties

Property code	Value	Unit	Source
gf	160.04	kJ/mol	Joback Method
hf	-187.29	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	54.31	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.365		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
tb	605.78	K	Joback Method
tc	809.13	K	Joback Method
tf	289.06	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.98	J/mol×K	605.78	Joback Method
cpg	566.60	J/mol×K	639.67	Joback Method
cpg	585.22	J/mol×K	673.56	Joback Method
cpg	602.85	J/mol×K	707.45	Joback Method
cpg	619.54	J/mol×K	741.34	Joback Method
cpg	635.30	J/mol×K	775.23	Joback Method
cpg	650.17	J/mol×K	809.13	Joback Method
dvisc	0.0030834	Pa×s	289.06	Joback Method
dvisc	0.0011724	Pa×s	341.85	Joback Method

dvisc	0.0005774	Pa×s	394.63	Joback Method
dvisc	0.0003361	Pa×s	447.42	Joback Method
dvisc	0.0002193	Pa×s	500.21	Joback Method
dvisc	0.0001553	Pa×s	552.99	Joback Method
dvisc	0.0001167	Pa×s	605.78	Joback Method

Sources

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=C6319853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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