

Benzene, 1,3-diisopropyl-5-propyl

Inchi:	InChI=1S/C15H24/c1-6-7-13-8-14(11(2)3)10-15(9-13)12(4)5/h8-12H,6-7H2,1-5H3
InchiKey:	ITIJRGPJXYLXNV-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CCc1cc(C(C)C)cc(C(C)C)c1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	163.69	kJ/mol	Joback Method
hf	-149.90	kJ/mol	Joback Method
hfus	20.82	kJ/mol	Joback Method
hvap	51.81	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.886		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
ripol	1549.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1513.00		NIST Webbook
tb	578.36	K	Joback Method
tc	779.69	K	Joback Method
tf	280.27	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.12	J/molxK	578.36	Joback Method
cpg	513.10	J/molxK	611.91	Joback Method

cpg	531.10	J/mol×K	645.47	Joback Method
cpg	548.15	J/mol×K	679.02	Joback Method
cpg	564.29	J/mol×K	712.58	Joback Method
cpg	579.54	J/mol×K	746.13	Joback Method
cpg	593.95	J/mol×K	779.69	Joback Method
dvisc	0.0033435	Paxs	280.27	Joback Method
dvisc	0.0013204	Paxs	329.95	Joback Method
dvisc	0.0006650	Paxs	379.63	Joback Method
dvisc	0.0003925	Paxs	429.31	Joback Method
dvisc	0.0002585	Paxs	479.00	Joback Method
dvisc	0.0001841	Paxs	528.68	Joback Method
dvisc	0.0001390	Paxs	578.36	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=R548835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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