

1,3,5-Trimethyl-2,6-di(cyclopentyl)benzene

Other names:	2,4-dicyclopentyl-1,3,5-trimethylbenzene
Inchi:	InChI=1S/C19H28/c1-13-12-14(2)19(17-10-6-7-11-17)15(3)18(13)16-8-4-5-9-16/h12,16-
InchiKey:	RXLACTJALSDWAX-UHFFFAOYSA-N
Formula:	C19H28
SMILES:	<chem>Cc1cc(C)c(C2CCCC2)c(C)c1C1CCCC1</chem>
Mol. weight [g/mol]:	256.43
CAS:	94440-26-3

Physical Properties

Property code	Value	Unit	Source
gf	256.09	kJ/mol	Joback Method
hf	-123.88	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	63.33	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.927		Crippen Method
mcvol	233.090	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
tb	711.28	K	Joback Method
tc	946.83	K	Joback Method
tf	402.19	K	Joback Method
vc	0.874	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.68	J/molxK	711.28	Joback Method
cpg	719.46	J/molxK	750.54	Joback Method
cpg	741.58	J/molxK	789.80	Joback Method
cpg	762.15	J/molxK	829.06	Joback Method
cpg	781.23	J/molxK	868.32	Joback Method
cpg	798.92	J/molxK	907.58	Joback Method
cpg	815.27	J/molxK	946.83	Joback Method
dvisc	0.0015249	Paxs	402.19	Joback Method

dvisc	0.0009305	Paxs	453.70	Joback Method
dvisc	0.0006280	Paxs	505.22	Joback Method
dvisc	0.0004558	Paxs	556.74	Joback Method
dvisc	0.0003493	Paxs	608.25	Joback Method
dvisc	0.0002790	Paxs	659.76	Joback Method
dvisc	0.0002303	Paxs	711.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C94440263&Units=SI

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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