1,3-di-isobutylmesitylene

Inchi: InChI=1S/C17H28/c1-11(2)8-16-13(5)10-14(6)17(15(16)7)9-12(3)4/h10-12H,8-9H2,1-7H3
InchiKey: JOQYFRRUSWTDQJ-UHFFFAOYSA-N
Formula: C17H28
SMILES: Cc1cc(C)c(CC(C)C)c(C)c1CC(C)C
Mol. weight [g/mol]: 232.40

Physical Properties

Property code	Value	Unit	Source
gf	161.27	kJ/mol	Joback Method
hf	-214.12	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	57.58	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.009		Crippen Method
mcvol	226.630	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook
tb	634.08	K	Joback Method
tc	831.82	K	Joback Method
tf	327.85	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.46	J/mol×K	634.08	Joback Method
cpg	619.86	J/mol×K	667.04	Joback Method
cpg	638.32	J/mol×K	699.99	Joback Method
cpg	655.84	J/mol×K	732.95	Joback Method
cpg	672.47	J/mol×K	765.90	Joback Method
cpg	688.22	J/mol×K	798.86	Joback Method
cpg	703.11	J/mol×K	831.82	Joback Method
dvisc	0.0016354	Pa×s	327.85	Joback Method

dvisc	0.0007757	Pa×s	378.89	Joback Method
dvisc	0.0004393	Pa×s	429.93	Joback Method
dvisc	0.0002806	Pa×s	480.96	Joback Method
dvisc	0.0001954	Pa×s	532.00	Joback Method
dvisc	0.0001449	Pa×s	583.04	Joback Method
dvisc	0.0001128	Pa×s	634.08	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=R200776&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

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