sec-Butylmesitylene

Inchi: InChI=1S/C13H20/c1-6-10(3)13-11(4)7-9(2)8-12(13)5/h7-8,10H,6H2,1-5H3
InchiKey: MBHVKXAUTWSICQ-UHFFFAOYSA-N
Formula: C13H20
SMILES: CCC(C)c1c(C)cc(C)cc1C
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	139.66	kJ/mol	Joback Method
hf	-114.81	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	48.41	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.125		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
tb	538.02	K	Joback Method
tc	742.16	K	Joback Method
tf	285.25	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.67	J/mol×K	538.02	Joback Method
cpg	471.81	J/mol×K	708.14	Joback Method
cpg	457.94	J/mol×K	674.11	Joback Method
cpg	443.31	J/mol×K	640.09	Joback Method
cpg	427.91	J/mol×K	606.07	Joback Method
cpg	411.70	J/mol×K	572.04	Joback Method
cpg	484.95	J/mol×K	742.16	Joback Method
dvisc	0.0001676	Pa×s	538.02	Joback Method

dvisc	0.0002108	Pa×s	495.89	Joback Method
dvisc	0.0002766	Pa×s	453.76	Joback Method
dvisc	0.0003838	Pa×s	411.63	Joback Method
dvisc	0.0005738	Pa×s	369.51	Joback Method
dvisc	0.0009514	Pa×s	327.38	Joback Method
dvisc	0.0018315	Pa×s	285.25	Joback Method

Sources

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=R201100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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