

n-butylmesitylene

Inchi:	InChI=1S/C13H20/c1-5-6-7-13-11(3)8-10(2)9-12(13)4/h8-9H,5-7H2,1-4H3
InchiKey:	WGWIEEZKILSKOQ-UHFFFAOYSA-N
Formula:	C13H20
SMILES:	CCCCc1c(C)cc(C)cc1C
Mol. weight [g/mol]:	176.30

Physical Properties

Property code	Value	Unit	Source
gf	142.10	kJ/mol	Joback Method
hf	-109.53	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.954		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1368.00		NIST Webbook
tb	538.46	K	Joback Method
tc	738.32	K	Joback Method
tf	300.25	K	Joback Method
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.39	J/mol×K	538.46	Joback Method
cpg	411.00	J/mol×K	571.77	Joback Method
cpg	426.83	J/mol×K	605.08	Joback Method
cpg	441.90	J/mol×K	638.39	Joback Method
cpg	456.23	J/mol×K	671.70	Joback Method
cpg	469.84	J/mol×K	705.01	Joback Method
cpg	482.75	J/mol×K	738.32	Joback Method
dvisc	0.0014318	Paxs	300.25	Joback Method
dvisc	0.0008260	Paxs	339.95	Joback Method

dvisc	0.0005346	Paxs	379.65	Joback Method
dvisc	0.0003758	Paxs	419.36	Joback Method
dvisc	0.0002807	Paxs	459.06	Joback Method
dvisc	0.0002197	Paxs	498.76	Joback Method
dvisc	0.0001782	Paxs	538.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R200934&Units=SI
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

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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