Benzene, 1,2,5-trimethyl-3-propyl

Other names: 1,4,5-Trimethyl-3-Propylbenzene
Inchi: InChI=1S/C12H18/c1-5-6-12-8-9(2)7-10(3)11(12)4/h7-8H,5-6H2,1-4H3
InchiKey: FXNRGRCXYVLCQN-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCCc1cc(C)cc(C)c1C
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	133.68	kJ/mol	Joback Method
hf	-88.89	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	46.57	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.564		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
ripol	1513.30		NIST Webbook
ripol	1513.30		NIST Webbook
ripol	1513.00		NIST Webbook
tb	515.58	K	Joback Method
tc	718.31	K	Joback Method
tf	288.98	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.28	J/mol×K	515.58	Joback Method

cpg	363.09	J/mol×K	549.37	Joback Method
cpg	378.15	J/mol×K	583.16	Joback Method
cpg	392.49	J/mol×K	616.94	Joback Method
cpg	406.14	J/mol×K	650.73	Joback Method
cpg	419.10	J/mol×K	684.52	Joback Method
cpg	431.41	J/mol×K	718.31	Joback Method
dvisc	0.0013949	Pa×s	288.98	Joback Method
dvisc	0.0008227	Pa×s	326.75	Joback Method
dvisc	0.0005414	Pa×s	364.51	Joback Method
dvisc	0.0003853	Pa×s	402.28	Joback Method
dvisc	0.0002908	Pa×s	440.05	Joback Method
dvisc	0.0002294	Pa×s	477.81	Joback Method
dvisc	0.0001874	Pa×s	515.58	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=R42885&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume