BENZENE, 1,3,5-TRIMETHYL-2-(1-METHYLETHENYL)-

Inchi: InChI=1S/C12H16/c1-8(2)12-10(4)6-9(3)7-11(12)5/h6-7H,1H2,2-5H3
InchiKey: KNMWUHBKZHDEOQ-UHFFFAOYSA-N
Formula: C12H16
SMILES: C=C(C)c1c(C)cc(C)cc1C
Mol. weight [g/mol]: 160.26

Physical Properties

Property code	Value	Unit	Source
af	0.4583		Cheméo Relay (1.0)
gf	212.97	kJ/mol	Joback Method
hf	57.14	kJ/mol	Cheméo Relay (1.0)
hfus	17.12	kJ/mol	Joback Method
hvap	57.64	kJ/mol	Cheméo Relay (1.0)
ie	7.98	eV	Cheméo Relay (1.0)
log10ws	-4.13		Cheméo Relay (1.0)
logp	3.645		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1311.00		NIST Webbook
tb	484.30 ± 0.20	K	NIST Webbook
tc	699.31	K	Cheméo Relay (1.0)
tf	241.55 ± 0.20	K	NIST Webbook
vc	0.559	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.63	J/mol×K	512.14	Joback Method
cpg	344.06	J/mol×K	547.30	Joback Method
cpg	358.70	J/mol×K	582.47	Joback Method
cpg	372.59	J/mol×K	617.63	Joback Method
cpg	385.75	J/mol×K	652.79	Joback Method
cpg	398.20	J/mol×K	687.96	Joback Method
cpg	409.97	J/mol×K	723.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14679131&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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