Benzene, (2,4-dimethylpentyl)-

Inchi: InChI=1S/C13H20/c1-11(2)9-12(3)10-13-7-5-4-6-8-13/h4-8,11-12H,9-10H2,1-3H3
InchiKey: QXXSGHXNHITGDL-UHFFFAOYSA-N
Formula: C13H20
SMILES: CC(C)CC(C)Cc1ccccc1
Mol. weight [g/mol]: 176.30
CAS: 54518-00-2

Physical Properties

Property code	Value	Unit	Source
chl	-7343.00	kJ/mol	NIST Webbook
gf	166.11	kJ/mol	Joback Method
hf	-85.68	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.911		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1247.00		NIST Webbook
tb	492.16 ± 0.30	K	NIST Webbook
tb	492.16 ± 0.30	K	NIST Webbook
tc	727.89	K	Joback Method
tf	232.69	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.25	J/mol×K	522.64	Joback Method
cpg	411.73	J/mol×K	556.85	Joback Method
cpg	429.19	J/mol×K	591.06	Joback Method
cpg	445.65	J/mol×K	625.26	Joback Method
cpg	461.16	J/mol×K	659.47	Joback Method
cpg	475.77	J/mol×K	693.68	Joback Method

cpg	489.50	J/mol×K	727.89	Joback Method
dvisc	0.0086915	Pa×s	232.69	Joback Method
dvisc	0.0025797	Pa×s	281.01	Joback Method
dvisc	0.0010936	Pa×s	329.34	Joback Method
dvisc	0.0005775	Pa×s	377.66	Joback Method
dvisc	0.0003525	Pa×s	425.99	Joback Method
dvisc	0.0002379	Pa×s	474.31	Joback Method
dvisc	0.0001727	Pa×s	522.64	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=C54518002&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
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