Benzene, 1-methyl-3-octyl

Inchi: InChI=1S/C15H24/c1-3-4-5-6-7-8-11-15-12-9-10-14(2)13-15/h9-10,12-13H,3-8,11H2,1-2
InchiKey: QMUTZNRXAKMEBK-UHFFFAOYSA-N
Formula: C15H24
SMILES: CCCCCCCCc1cccc(C)c1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	178.20	kJ/mol	Joback Method
hf	-127.87	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.898		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
ripol	1550.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1552.00		NIST Webbook
tb	574.26	K	Joback Method
tc	766.81	K	Joback Method
tf	297.75	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.06	J/mol×K	574.26	Joback Method
cpg	576.06	J/mol×K	734.72	Joback Method
cpg	561.18	J/mol×K	702.63	Joback Method
cpg	545.48	J/mol×K	670.54	Joback Method
cpg	528.91	J/mol×K	638.44	Joback Method
cpg	511.45	J/mol×K	606.35	Joback Method

cpg	590.13	J/mol×K	766.81	Joback Method
dvisc	0.0001620	Pa×s	574.26	Joback Method
dvisc	0.0002099	Pa×s	528.17	Joback Method
dvisc	0.0002857	Pa×s	482.09	Joback Method
dvisc	0.0004153	Pa×s	436.00	Joback Method
dvisc	0.0006592	Pa×s	389.92	Joback Method
dvisc	0.0011846	Pa×s	343.83	Joback Method
dvisc	0.0025521	Pa×s	297.75	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R550100&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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