Benzene, (1,1-diethylpropyl)-

Other names: (1,1-Diethylpropyl)benzene
Inchi: InChI=1S/C13H20/c1-4-13(5-2,6-3)12-10-8-7-9-11-12/h7-11H,4-6H2,1-3H3
InchiKey: WLVNEALRNQEPMS-UHFFFAOYSA-N
Formula: C13H20
SMILES: CCC(CC)(CC)c1ccccc1
Mol. weight [g/mol]: 176.30
CAS: 4170-84-7

Physical Properties

Property code	Value	Unit	Source
gf	173.83	kJ/mol	Joback Method
hf	-83.87	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.154		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
tb	520.29	K	Joback Method
tc	729.27	K	Joback Method
tf	294.27 ± 0.50	K	NIST Webbook
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.64	J/mol×K	520.29	Joback Method
cpg	414.50	J/mol×K	555.12	Joback Method
cpg	432.19	J/mol×K	589.95	Joback Method
cpg	448.75	J/mol×K	624.78	Joback Method
cpg	464.27	J/mol×K	659.61	Joback Method

cpg	478.79	J/mol×K	694.44	Joback Method
cpg	492.37	J/mol×K	729.27	Joback Method
dvisc	0.0052309	Pa×s	265.11	Joback Method
dvisc	0.0020371	Pa×s	307.64	Joback Method
dvisc	0.0009975	Pa×s	350.17	Joback Method
dvisc	0.0005702	Pa×s	392.70	Joback Method
dvisc	0.0003636	Pa×s	435.23	Joback Method
dvisc	0.0002511	Pa×s	477.76	Joback Method
dvisc	0.0001843	Pa×s	520.29	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=C4170847&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume