

Benzene, 1-(1-ethylpropyl)-3-(1-methylbutyl)-

Inchi:	InChI=1S/C16H26/c1-5-9-13(4)15-10-8-11-16(12-15)14(6-2)7-3/h8,10-14H,5-7,9H2,1-4H
InchiKey:	LJXJIIICRXIAWQR-UHFFFAOYSA-N
Formula:	C16H26
SMILES:	CCCC(C)c1cccc(C(CC)CC)c1
Mol. weight [g/mol]:	218.38
CAS:	100945-39-9

Physical Properties

Property code	Value	Unit	Source
gf	181.74	kJ/mol	Joback Method
hf	-159.07	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.494		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
tb	596.26	K	Joback Method
tc	793.83	K	Joback Method
tf	279.02	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.90	J/molxK	596.26	Joback Method
cpg	634.22	J/molxK	760.90	Joback Method
cpg	618.49	J/molxK	727.97	Joback Method
cpg	601.82	J/molxK	695.05	Joback Method
cpg	584.20	J/molxK	662.12	Joback Method
cpg	565.57	J/molxK	629.19	Joback Method
cpg	649.07	J/molxK	793.83	Joback Method
dvisc	0.0001293	Paxs	596.26	Joback Method
dvisc	0.0001756	Paxs	543.39	Joback Method

dvisc	0.0002546	Paxs	490.51	Joback Method
dvisc	0.0004041	Paxs	437.64	Joback Method
dvisc	0.0007280	Paxs	384.77	Joback Method
dvisc	0.0015822	Paxs	331.89	Joback Method
dvisc	0.0046147	Paxs	279.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C100945399&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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