

Benzene, 1-ethyl-2-octyl

Inchi:	InChI=1S/C16H26/c1-3-5-6-7-8-9-13-16-14-11-10-12-15(16)4-2/h10-12,14H,3-9,13H2,1-
InchiKey:	HUNNCGSXMVRWHS-UHFFFAOYSA-N
Formula:	C16H26
SMILES:	CCCCCCCCc1ccccc1CC
Mol. weight [g/mol]:	218.38

Physical Properties

Property code	Value	Unit	Source
gf	186.62	kJ/mol	Joback Method
hf	-148.51	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	54.15	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.152		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1595.00		NIST Webbook
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tb	597.14	K	Joback Method
tc	787.38	K	Joback Method
tf	309.02	K	Joback Method
vc	0.824	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.23	J/mol×K	597.14	Joback Method
cpg	630.29	J/mol×K	755.67	Joback Method
cpg	615.03	J/mol×K	723.97	Joback Method
cpg	598.94	J/mol×K	692.26	Joback Method
cpg	581.96	J/mol×K	660.55	Joback Method
cpg	564.07	J/mol×K	628.85	Joback Method
cpg	644.73	J/mol×K	787.38	Joback Method
dvisc	0.0001482	Paxs	597.14	Joback Method

dvisc	0.0001929	Paxs	549.12	Joback Method
dvisc	0.0002641	Paxs	501.10	Joback Method
dvisc	0.0003863	Paxs	453.08	Joback Method
dvisc	0.0006186	Paxs	405.06	Joback Method
dvisc	0.0011242	Paxs	357.04	Joback Method
dvisc	0.0024600	Paxs	309.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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

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