BENZENE, (1-ETHYLHEPTYL)-

Inchi: InChI=1S/C15H24/c1-3-5-6-8-11-14(4-2)15-12-9-7-10-13-15/h7,9-10,12-14H,3-6,8,11H2,
InchiKey: YXIUVYKXVOKDQS-UHFFFAOYSA-N
Formula: C15H24
SMILES: CCCCCCC(CC)c1ccccc1
Mol. weight [g/mol]: 204.36

Physical Properties

Property code	Value	Unit	Source
af	0.5371		Cheméo Relay (1.0)
hf	-101.64	kJ/mol	Cheméo Relay (1.0)
hfus	25.12	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-5.91		Cheméo Relay (1.0)
logp	5.151		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1460.00		NIST Webbook
tb	534.61	K	Cheméo Relay (1.0)
tc	734.94	K	Cheméo Relay (1.0)
tf	237.55	K	Cheméo Relay (1.0)
vc	0.733	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.85	J/mol×K	568.84	Joback Method
cpg	592.90	J/mol×K	764.22	Joback Method
cpg	578.50	J/mol×K	731.66	Joback Method
cpg	563.24	J/mol×K	699.10	Joback Method
cpg	547.09	J/mol×K	666.53	Joback Method
cpg	530.00	J/mol×K	633.97	Joback Method
cpg	511.93	J/mol×K	601.40	Joback Method
dvisc	0.0004766	Pa×s	419.53	Joback Method

dvisc	0.0001551	Pa×s	568.84	Joback Method
dvisc	0.0002099	Pa×s	519.07	Joback Method
dvisc	0.0003028	Pa×s	469.30	Joback Method
dvisc	0.0050617	Pa×s	270.23	Joback Method
dvisc	0.0008475	Pa×s	369.77	Joback Method
dvisc	0.0018025	Pa×s	320.00	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20216879&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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