Benzene, 1-heptyl-2-propyl

Inchi: InChI=1S/C16H26/c1-3-5-6-7-8-12-16-14-10-9-13-15(16)11-4-2/h9-10,13-14H,3-8,11-12H
InchiKey: INGLFYYOAQSFKI-UHFFFAOYSA-N
Formula: C16H26
SMILES: CCCCCCCc1ccccc1CCC
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	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	597.14	K	Joback Method
tc	787.38	K	Joback Method
tf	309.02	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0024600	Pa×s	309.02	Joback Method
dvisc	0.0011242	Pa×s	357.04	Joback Method
dvisc	0.0006186	Pa×s	405.06	Joback Method
dvisc	0.0003863	Pa×s	453.08	Joback Method
dvisc	0.0002641	Pa×s	501.10	Joback Method
dvisc	0.0001929	Pa×s	549.12	Joback Method
dvisc	0.0001482	Pa×s	597.14	Joback Method

Sources

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=R13688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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