

Benzene, 1-heptyl-4-propyl

Inchi:	InChI=1S/C16H26/c1-3-5-6-7-8-10-16-13-11-15(9-4-2)12-14-16/h11-14H,3-10H2,1-2H3
InchiKey:	KYAHMNFLQOYUTH-UHFFFAOYSA-N
Formula:	C16H26
SMILES:	CCCCCCCc1ccc(CCC)cc1
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
ripol	1830.90		NIST Webbook
ripol	1823.00		NIST Webbook
ripol	1823.00		NIST Webbook
ripol	1823.00		NIST Webbook
ripol	1830.90		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/molxK	597.14	Joback Method
cpg	630.29	J/molxK	755.67	Joback Method
cpg	615.03	J/molxK	723.97	Joback Method
cpg	598.94	J/molxK	692.26	Joback Method
cpg	581.96	J/molxK	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

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=R12622&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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