

2-ethyl-6-methylnaphthalene

Inchi:	InChI=1S/C13H14/c1-3-11-5-7-12-8-10(2)4-6-13(12)9-11/h4-9H,3H2,1-2H3
InchiKey:	ZOYUJOHRFWIQTH-UHFFFAOYSA-N
Formula:	C13H14
SMILES:	CCc1ccc2cc(C)ccc2c1
Mol. weight [g/mol]:	170.25
CAS:	7372-86-3

Physical Properties

Property code	Value	Unit	Source
af	0.4880		KDB
gf	258.38	kJ/mol	Joback Method
hf	93.01	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	49.77	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.711		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2710.00	kPa	KDB
tb	543.20	K	KDB
tc	766.60	K	KDB
tf	318.00	K	KDB
vc	0.578	m ³ /kmol	KDB
zc	0.2455360		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.22	J/mol×K	552.46	Joback Method
cpg	357.89	J/mol×K	590.33	Joback Method
cpg	372.52	J/mol×K	628.20	Joback Method
cpg	386.18	J/mol×K	666.07	Joback Method
cpg	398.93	J/mol×K	703.95	Joback Method
cpg	410.84	J/mol×K	741.82	Joback Method
cpg	421.96	J/mol×K	779.69	Joback Method

dvisc	0.0013320	Paxs	320.43	Joback Method
dvisc	0.0008996	Paxs	359.10	Joback Method
dvisc	0.0006558	Paxs	397.77	Joback Method
dvisc	0.0005056	Paxs	436.45	Joback Method
dvisc	0.0004066	Paxs	475.12	Joback Method
dvisc	0.0003379	Paxs	513.79	Joback Method
dvisc	0.0002882	Paxs	552.46	Joback Method

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol785.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7372863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
zc:	Critical Compressibility

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