2-ethyl-3-methylnaphthalene

Inchi: InChI=1S/C13H14/c1-3-11-9-13-7-5-4-6-12(13)8-10(11)2/h4-9H,3H2,1-2H3
InchiKey: OKUXCOASJUSADT-UHFFFAOYSA-N
Formula: C13H14
SMILES: CCc1cc2ccccc2cc1C
Mol. weight [g/mol]: 170.25
CAS: 31032-94-7

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	550.20	K	KDB
tc	776.40	K	KDB
tf	344.00	K	KDB
vc	0.578	m3/kmol	KDB
zc	0.2424370		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	Pa×s	320.43	Joback Method
dvisc	0.0008996	Pa×s	359.10	Joback Method
dvisc	0.0006558	Pa×s	397.77	Joback Method
dvisc	0.0005056	Pa×s	436.45	Joback Method
dvisc	0.0004066	Pa×s	475.12	Joback Method
dvisc	0.0003379	Pa×s	513.79	Joback Method
dvisc	0.0002882	Pa×s	552.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31032947&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol784.mol

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