1,2-Diethoxy-3-ethylbenzene

Other names: Benzene, 1,2-diethoxy-3-ethyl
Inchi: InChI=1S/C12H18O2/c1-4-10-8-7-9-11(13-5-2)12(10)14-6-3/h7-9H,4-6H2,1-3H3
InchiKey: FAZOHODJTTYSEH-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CCOc1cccc(CC)c1OCC
Mol. weight [g/mol]: 194.27
CAS: 131358-05-9

Physical Properties

Property code	Value	Unit	Source
gf	-66.69	kJ/mol	Joback Method
hf	-341.86	kJ/mol	Joback Method
hfus	22.47	kJ/mol	Joback Method
hvap	50.73	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.046		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook
tb	555.44	K	Joback Method
tc	753.59	K	Joback Method
tf	320.92	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.67	J/mol×K	555.44	Joback Method
cpg	469.46	J/mol×K	720.57	Joback Method
cpg	456.65	J/mol×K	687.54	Joback Method
cpg	443.16	J/mol×K	654.52	Joback Method
cpg	429.00	J/mol×K	621.49	Joback Method
cpg	414.17	J/mol×K	588.47	Joback Method

cpg	481.59	J/mol×K	753.59	Joback Method
dvisc	0.0001336	Pa×s	555.44	Joback Method
dvisc	0.0001666	Pa×s	516.35	Joback Method
dvisc	0.0002152	Pa×s	477.27	Joback Method
dvisc	0.0002910	Pa×s	438.18	Joback Method
dvisc	0.0004176	Pa×s	399.09	Joback Method
dvisc	0.0006481	Pa×s	360.01	Joback Method
dvisc	0.0011194	Pa×s	320.92	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=C131358059&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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