1,2,3-Trimethyl-4-Ethylbenzene

Other names: Benzene, 1,2,3-trimethyl-4-ethyl
Benzene, 1-ethyl-2,3,4-trimethyl-
Inchi: InChI=1S/C11H16/c1-5-11-7-6-8(2)9(3)10(11)4/h6-7H,5H2,1-4H3
InchiKey: BAMWORSGQSUNSC-UHFFFAOYSA-N
Formula: C11H16
SMILES: CCc1ccc(C)c(C)c1C
Mol. weight [g/mol]: 148.24
CAS: 61827-86-9

Physical Properties

Property code	Value	Unit	Source
gf	125.26	kJ/mol	Joback Method
hf	-68.25	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.174		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1222.00		NIST Webbook
rinpol	1222.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1503.80		NIST Webbook
tb	492.70	K	Joback Method
tc	698.35	K	Joback Method
tf	277.71	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.04	J/mol×K	492.70	Joback Method

cpg	316.91	J/mol×K	526.98	Joback Method
cpg	331.09	J/mol×K	561.25	Joback Method
cpg	344.60	J/mol×K	595.53	Joback Method
cpg	357.45	J/mol×K	629.80	Joback Method
cpg	369.67	J/mol×K	664.08	Joback Method
cpg	381.26	J/mol×K	698.35	Joback Method
dvisc	0.0013334	Pa×s	277.71	Joback Method
dvisc	0.0008052	Pa×s	313.54	Joback Method
dvisc	0.0005392	Pa×s	349.37	Joback Method
dvisc	0.0003891	Pa×s	385.21	Joback Method
dvisc	0.0002967	Pa×s	421.04	Joback Method
dvisc	0.0002362	Pa×s	456.87	Joback Method
dvisc	0.0001943	Pa×s	492.70	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61827869&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume