

Benzene, 1-ethyl-3-isocyanato-

Other names:	3-ethylphenyl isocyanate
Inchi:	InChI=1S/C9H9NO/c1-2-8-4-3-5-9(6-8)10-7-11/h3-6H,2H2,1H3
InchiKey:	DNFZCDLEGMEKMI-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	CCc1cccc(N=C=O)c1
Mol. weight [g/mol]:	147.18
CAS:	23138-58-1

Physical Properties

Property code	Value	Unit	Source
af	0.4733		Cheméo Relay (1.0)
gf	117.06	kJ/mol	Cheméo Relay (1.0, beta)
hf	-29.87	kJ/mol	Cheméo Relay (1.0)
hvap	52.34	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
logp	2.216		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	465.97	K	Cheméo Relay (1.0)
tc	699.21	K	Cheméo Relay (1.0)
tf	227.93	K	Cheméo Relay (1.0)
vc	0.434	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51367e+01
Coeff. B	-4.24003e+03
Coeff. C	-7.73230e+01
Temperature range (K), min.	362.87
Temperature range (K), max.	508.87

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23138581&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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