Benzene, (2-isothiocyanatoethyl)-

Other names:	Isothiocyanic acid, phenethyl ester
	«beta»-Phenethyl isothiocyanate
	«beta»-Phenylethyl isothiocyanate
	Phenethyl isothiocyanate
	Phenethyl mustard oil
	Phenylethyl isothiocyanate
	Phenylethyl mustard oil
	2-Phenylethyl isothiocyanate
	Isothiocyanic acid «beta»-phenylethyl ester
	Phenylaethylsenfoel
	NSC 87868
Inchi:	InChI=1S/C9H9NS/c11-8-10-7-6-9-4-2-1-3-5-9/h1-5H,6-7H2
InchiKey:	IZJDOKYDEWTZSO-UHFFFAOYSA-N
Formula:	C9H9NS
SMILES:	S=C=NCCc1ccccc1
Mol. weight [g/mol]:	163.24
CAS:	2257-09-2

Physical Properties

Property code	Value	Unit	Source
hf	291.51	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.332		Crippen Method
mcvol	131.640	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1472.10		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1465.00		NIST Webbook

ripol	2234.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2216.00		NIST Webbook
ripol	2234.00		NIST Webbook
tb	577.95	K	Joback Method
tc	831.91	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2257092&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

hf:	Enthalpy of formation 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

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