

2-Ethylthiacyclohexane

Other names:	2-Ethylthiane 2-Ethylthiapyran
Inchi:	InChI=1S/C7H14S/c1-2-7-5-3-4-6-8-7/h7H,2-6H2,1H3
InchiKey:	GYIFZSXJAVPBL-LUHFFFAOYSA-N
Formula:	C7H14S
SMILES:	CCC1CCCCS1
Mol. weight [g/mol]:	130.25
CAS:	1613-52-1

Physical Properties

Property code	Value	Unit	Source
gf	72.37	kJ/mol	Joback Method
hf	-88.23	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	37.42	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.682		Crippen Method
mcpvol	114.980	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1011.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1019.00		NIST Webbook
tb	426.94	K	Joback Method
tc	646.42	K	Joback Method
tf	259.48	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.37	J/mol×K	426.94	Joback Method

cpg	236.92	J/mol×K	463.52	Joback Method
cpg	252.59	J/mol×K	500.10	Joback Method
cpg	267.39	J/mol×K	536.68	Joback Method
cpg	281.37	J/mol×K	573.26	Joback Method
cpg	294.54	J/mol×K	609.84	Joback Method
cpg	306.93	J/mol×K	646.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.16872e+01
Coeff. B	-2.85803e+03
Coeff. C	-5.98390e+01
Temperature range (K), min.	310.55
Temperature range (K), max.	508.11

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C1613521&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
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
pvap:	Vapor 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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