

2-ethyl-(2H)-thiapyran

Other names:	2-Ethyl-2H-thiapyrane
Inchi:	InChI=1S/C7H10S/c1-2-7-5-3-4-6-8-7/h3-7H,2H2,1H3
InchiKey:	GQGPAOVRSUWPSI-UHFFFAOYSA-N
Formula:	C7H10S
SMILES:	CCC1C=CC=CS1
Mol. weight [g/mol]:	126.22

Physical Properties

Property code	Value	Unit	Source
gf	132.29	kJ/mol	Joback Method
hf	27.33	kJ/mol	Joback Method
hfus	11.82	kJ/mol	Joback Method
hvap	38.00	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.582		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	1022.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1019.00		NIST Webbook
ripol	1394.00		NIST Webbook
tb	425.26	K	Joback Method
tc	649.53	K	Joback Method
tf	261.00	K	Joback Method
vc	0.379	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.76	J/mol×K	425.26	Joback Method
cpg	206.55	J/mol×K	462.64	Joback Method
cpg	219.52	J/mol×K	500.02	Joback Method

cpg	231.70	J/mol×K	537.40	Joback Method
cpg	243.12	J/mol×K	574.77	Joback Method
cpg	253.81	J/mol×K	612.15	Joback Method
cpg	263.80	J/mol×K	649.53	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=R194666&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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

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