2-(propylthio)ethylamine

Inchi: InChI=1S/C5H13NS/c1-2-4-7-5-3-6/h2-6H2,1H3
InchiKey: KHHKBTRFZTUVRD-UHFFFAOYSA-N
Formula: C5H13NS
SMILES: CCCSCCN
Mol. weight [g/mol]: 119.23

Physical Properties

Property code	Value	Unit	Source
gf	90.79	kJ/mol	Joback Method
hf	-70.87	kJ/mol	Joback Method
hfus	18.03	kJ/mol	Joback Method
hvap	44.18	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.088		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
rinpol	1029.00		NIST Webbook
rinpol	1029.00		NIST Webbook
tb	455.11	K	Joback Method
tc	659.92	K	Joback Method
tf	263.77	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.88	J/mol×K	455.11	Joback Method
cpg	229.77	J/mol×K	489.25	Joback Method
cpg	240.18	J/mol×K	523.38	Joback Method
cpg	250.12	J/mol×K	557.52	Joback Method
cpg	259.59	J/mol×K	591.65	Joback Method
cpg	268.62	J/mol×K	625.79	Joback Method
cpg	277.19	J/mol×K	659.92	Joback Method

Sources

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=R231359&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/77-730-6/2-propylthio-ethylamine.pdf
Generated by Cheméo on 2024-04-27 14:01:31.555202941 +0000 UTC m=+16515740.475780252.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.