Acetamide, N-tetrahydrofurfuryl-2-phenylthio-

Inchi: InChI=1S/C13H17NO2S/c15-13(14-9-11-5-4-8-16-11)10-17-12-6-2-1-3-7-12/h1-3,6-7,11
InchiKey: HYFXXCQTXREDNT-UHFFFAOYSA-N
Formula: C13H17NO2S
SMILES: O=C(CSc1ccccc1)NCC1CCCO1
Mol. weight [g/mol]: 251.34

Physical Properties

Property code	Value	Unit	Source
gf	115.01	kJ/mol	Joback Method
hf	-163.88	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	71.57	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.074		Crippen Method
mcvol	193.180	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	738.57	K	Joback Method
tc	984.44	K	Joback Method
tf	437.15	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.79	J/mol×K	738.57	Joback Method
cpg	562.77	J/mol×K	779.55	Joback Method
cpg	577.37	J/mol×K	820.53	Joback Method
cpg	590.65	J/mol×K	861.51	Joback Method
cpg	602.70	J/mol×K	902.48	Joback Method
cpg	613.58	J/mol×K	943.46	Joback Method
cpg	623.36	J/mol×K	984.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307204&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

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