Acetamide, 2-(phenylthio)-N-butyl-N-ethyl-

Inchi: InChI=1S/C14H21NOS/c1-3-5-11-15(4-2)14(16)12-17-13-9-7-6-8-10-13/h6-10H,3-5,11-1
InchiKey: QISXQGYHBQANEF-UHFFFAOYSA-N
Formula: C14H21NOS
SMILES: CCCCN(CC)C(=O)CSc1ccccc1
Mol. weight [g/mol]: 251.39

Physical Properties

Property code	Value	Unit	Source
gf	194.39	kJ/mol	Joback Method
hf	-98.94	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.427		Crippen Method
mcvol	212.260	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
tb	681.49	K	Joback Method
tc	896.34	K	Joback Method
tf	390.76	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.70	J/mol×K	681.49	Joback Method
cpg	581.21	J/mol×K	717.30	Joback Method
cpg	596.61	J/mol×K	753.11	Joback Method
cpg	610.96	J/mol×K	788.91	Joback Method
cpg	624.29	J/mol×K	824.72	Joback Method
cpg	636.68	J/mol×K	860.53	Joback Method
cpg	648.15	J/mol×K	896.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415725&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