Acetamide, N-(1-naphthyl)-2-phenylthio-

Inchi: InChI=1S/C18H15NOS/c20-18(13-21-15-9-2-1-3-10-15)19-17-12-6-8-14-7-4-5-11-16(14)17
InchiKey: MEJSRRSAWKDLSH-UHFFFAOYSA-N
Formula: C18H15NOS
SMILES: O=C(CSc1ccccc1)Nc1cccc2ccccc12
Mol. weight [g/mol]: 293.38

Physical Properties

Property code	Value	Unit	Source
gf	416.11	kJ/mol	Joback Method
hf	220.57	kJ/mol	Joback Method
hfus	37.92	kJ/mol	Joback Method
hvap	82.52	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.571		Crippen Method
mcvol	225.400	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	2754.00		NIST Webbook
tb	861.38	K	Joback Method
tc	1126.65	K	Joback Method
tf	527.67	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.18	J/mol×K	861.38	Joback Method
cpg	645.33	J/mol×K	905.59	Joback Method
cpg	657.28	J/mol×K	949.80	Joback Method
cpg	668.19	J/mol×K	994.02	Joback Method
cpg	678.19	J/mol×K	1038.23	Joback Method
cpg	687.45	J/mol×K	1082.44	Joback Method
cpg	696.10	J/mol×K	1126.65	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307212&Units=SI

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