(Phenylthio)acetic acid, 1-naphthyl ester

Inchi: InChI=1S/C18H14O2S/c19-18(13-21-15-9-2-1-3-10-15)20-17-12-6-8-14-7-4-5-11-16(14)1
InchiKey: WRNQPKJZDDXTKR-UHFFFAOYSA-N
Formula: C18H14O2S
SMILES: O=C(CSc1ccccc1)Oc1cccc2ccccc12
Mol. weight [g/mol]: 294.37

Physical Properties

Property code	Value	Unit	Source
gf	221.72	kJ/mol	Joback Method
hf	34.88	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	78.49	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.537		Crippen Method
mcvol	221.290	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	2525.00		NIST Webbook
tb	833.63	K	Joback Method
tc	1098.93	K	Joback Method
tf	497.24	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.84	J/mol×K	833.63	Joback Method
cpg	620.38	J/mol×K	877.85	Joback Method
cpg	632.59	J/mol×K	922.06	Joback Method
cpg	643.58	J/mol×K	966.28	Joback Method
cpg	653.45	J/mol×K	1010.50	Joback Method
cpg	662.33	J/mol×K	1054.72	Joback Method
cpg	670.33	J/mol×K	1098.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308341&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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