N-phenyl-n'-p-carbethoxy phenyl thiocarbamide

Inchi: InChI=1S/C16H16N2O2S/c1-2-20-15(19)12-8-10-14(11-9-12)18-16(21)17-13-6-4-3-5-7-1

InchiKey: FUBMAKIAKSVODK-UHFFFAOYSA-N

Formula: C16H16N2O2S

SMILES: CCOC(=O)c1ccc(NC(=S)Nc2ccccc2)cc1

Mol. weight [g/mol]: 300.38

CAS: 1158-23-2

Physical Properties

Property code	Value	Unit	Source
gf	360.95	kJ/mol	Joback Method
hf	96.66	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.672		Crippen Method
mcvol	228.230	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
tb	870.49	K	Joback Method
tc	1117.98	K	Joback Method
tf	547.19	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.60	J/mol×K	870.49	Joback Method
cpg	657.83	J/mol×K	911.74	Joback Method
cpg	669.09	J/mol×K	952.99	Joback Method
cpg	679.50	J/mol×K	994.24	Joback Method
cpg	689.16	J/mol×K	1035.49	Joback Method
cpg	698.19	J/mol×K	1076.73	Joback Method
cpg	706.70	J/mol×K	1117.98	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=C1158232&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume