Phenylthioacetamide, N,N-didecyl-

Inchi: InChI=1S/C28H49NOS/c1-3-5-7-9-11-13-15-20-24-29(25-21-16-14-12-10-8-6-4-2)28(30)
InchiKey: BTROQBOSTNMHHP-UHFFFAOYSA-N
Formula: C28H49NOS
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)CSc1ccccc1
Mol. weight [g/mol]: 447.76

Physical Properties

Property code	Value	Unit	Source
gf	312.27	kJ/mol	Joback Method
hf	-387.90	kJ/mol	Joback Method
hfus	71.07	kJ/mol	Joback Method
hvap	95.80	kJ/mol	Joback Method
log10ws	-9.35		Crippen Method
logp	8.889		Crippen Method
mcvol	409.520	ml/mol	McGowan Method
pc	817.73	kPa	Joback Method
tb	1001.81	K	Joback Method
tc	1227.58	K	Joback Method
tf	548.54	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.99	J/mol×K	1001.81	Joback Method
cpg	1419.92	J/mol×K	1039.44	Joback Method
cpg	1438.44	J/mol×K	1077.07	Joback Method
cpg	1455.66	J/mol×K	1114.70	Joback Method
cpg	1471.70	J/mol×K	1152.33	Joback Method
cpg	1486.65	J/mol×K	1189.96	Joback Method
cpg	1500.64	J/mol×K	1227.58	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=U308167&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume